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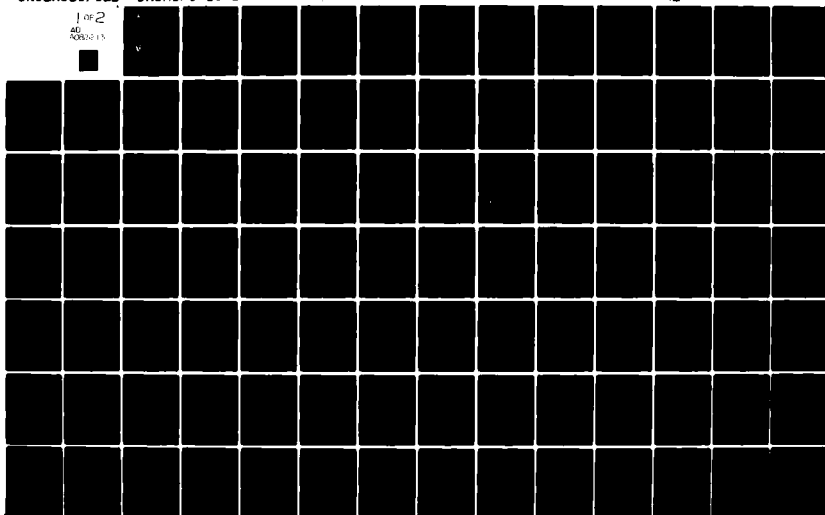
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TECHNICAL REPORT O-80-1

**A COMPUTER EXPERIMENT TO INVESTIGATE  
THE EFFECT OF DIFFERENTIAL DIFFUSION ON  
SMOKE MODELING CALCULATIONS**

Bruce W. Fowler  
Thomas B. Owens  
Advanced Systems Concepts Office  
US Army Missile Command

18 October 1979

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**U.S. ARMY MISSILE COMMAND**

**Redstone Arsenal, Alabama 35809**

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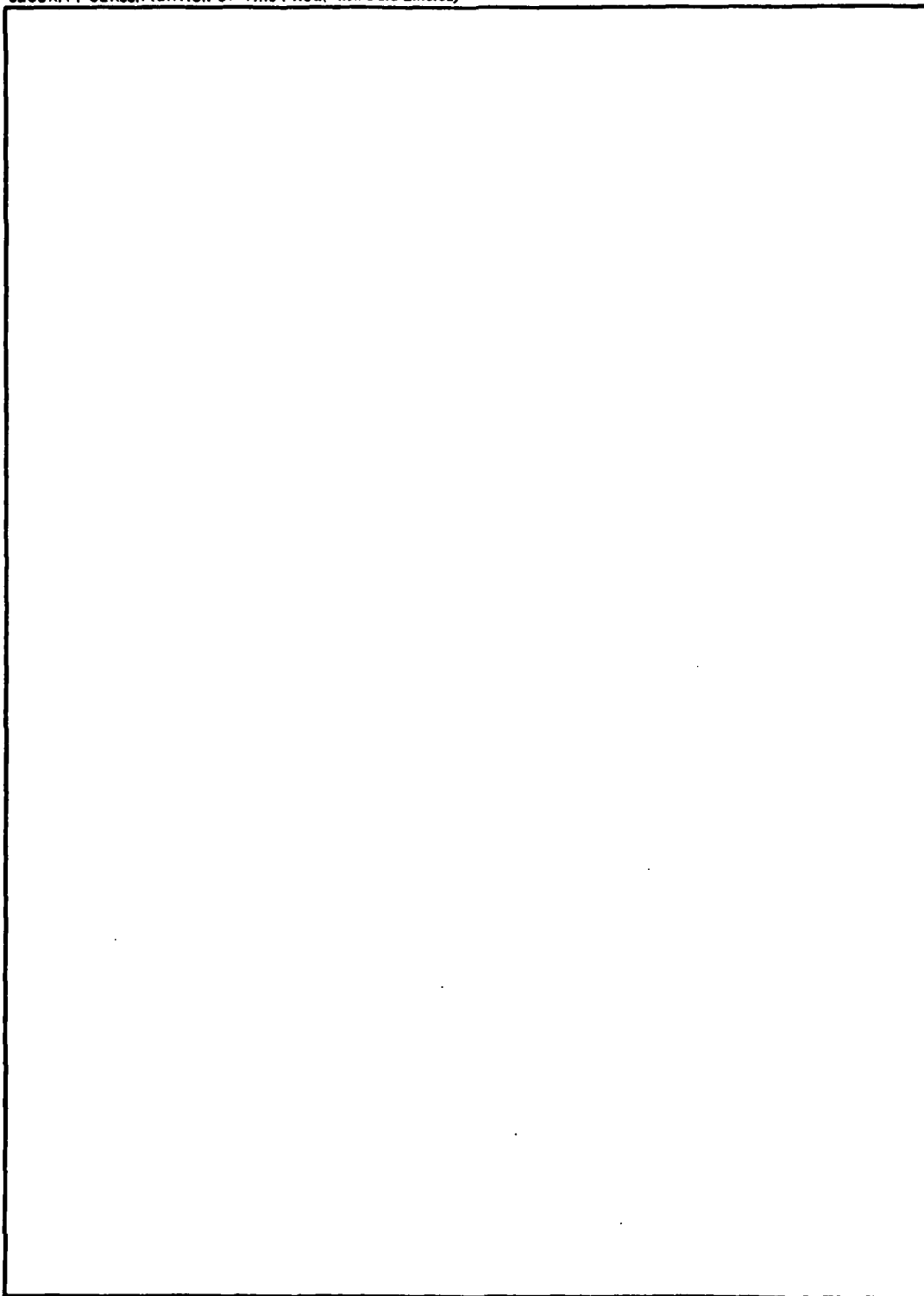
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## I. INTRODUCTION

This report describes a numerical experiment conducted to investigate the constraints placed on smoke modeling by a common assumption. That assumption, known as separability [1], ignores the differential diffusion properties of a polydisperse aerosol for simplicity.

In this experiment, the consequences of this assumption were examined. Idealized, spherical aerosols of known source particle size distribution were allowed to differentially diffuse in a Fickian manner. To avoid geometric confusion, spherical symmetry was assumed. Additionally, the separability assumption was applied for average particle sizes corresponding to the first three moments of the source particle size distribution. Calculations were then made at selected points and times within the aerosol cloud of total concentration, extinction coefficient, optical depth, and transmission.

The results of these calculations were then compared to assess the impact of the separability assumption on the accuracy of smoke modeling. The theory of the experiment is developed in Sections II and III. The conduct of the experiment is described and the results presented and discussed in Section IV. Conclusions are presented in Section V.

This experiment is part of an on-going examination of the effect of battlefield obscuration on the performance of missile weapons systems as part of the Concepts Analysis and Validation work area of the A214 Missile Technology Program. The results of this experiment will be used in the formulation, analysis, and evaluation of present and conceptual missile weapon systems.

## II. TRANSPORT AND DIFFUSION

The transport and diffusion of a smoke cloud is usually modeled under the assumption of separability [1]. This assumption allows the particle concentration - size distribution function  $N(r, \underline{R})$  where  $r$  is the particle radius and  $\underline{R}$  is position and time (four vector) to be separated in the form

$$N(r, \underline{R}) = n(r) C(\underline{R}) \quad (1)$$

where:  $n(r)$  = particle size distribution function, and  
 $C(\underline{R})$  = particle concentration function.

Normally,  $N(r, \underline{R})$  has units of number per volume per radius while  $n(r)$  has units of number per mass per radius, and  $C(\underline{R})$  has units of mass per volume.

The extinction coefficient  $\alpha(\underline{R})$  (units of reciprocal length) has the form

$$\alpha(\underline{R}) = \int_0^{\infty} N(r, \underline{R}) \sigma(r) dr, \quad (2)$$

where  $\sigma(r)$  is the extinction cross section, usually calculated using Mie theory [2]. In practice, Equation (2) is approximated as

$$\alpha(\underline{R}) \cong \int_{r_1}^{r_2} N(r, \underline{R}) \sigma(r) dr \quad (3)$$

since only those particles of appreciable extinction cross section or hydrodynamic size are measurable.

Equation (3) may be combined with Equation (1) to yield the average  $\langle \alpha(\underline{R}) \rangle$ ,

$$\langle \alpha(\underline{R}) \rangle \cong \int_{r_1}^{r_2} n(r) C(\underline{R}) \sigma(r) dr \quad (4a)$$

$$= C(\underline{R}) \alpha \quad (4b)$$

where:

$$\alpha \equiv \int_{r_1}^{r_2} n(r) \sigma(r) dr.$$

This is the profit of the separability approximation; the specific cross section,  $\alpha$ , is a constant within the cloud.

The particle concentration function  $C(\underline{R})$  is frequently modeled by trivariate gaussian function that are approximate solutions of the diffusion equation,

$$\frac{dC}{dt} = D \nabla^2 C \quad (5)$$

Equation (5) is appropriate for isotropic diffusion along streamlines and is much simpler than the diffusion equation normally used. For the purposes of this experiment, however, it will suffice. The parameter D, the diffusion coefficient, is a function of several factors, including the particle radius. (See Reference 3 ) The form of D is

$$D = \frac{kTg}{6\pi\mu r} \quad (6)$$

where

- $k$  = Boltzman's constant,
- $T$  = absolute temperature,
- $\mu$  = viscosity of air, and
- $g = 1 + \ell/r (A_1 + A_2 \exp(-2A_3 r/\ell))$
- $\ell$  = mean free path of air molecules
- $A_i$  = empirical constants
- $A_1 = 1,257,$
- $A_2 = 0.400,$  and
- $A_3 = 0.500.$

(7)

Equation (7) may be seen to be a function of temperature and particle radius. Temperature is commonly considered in the modeling of smoke; particle radius is not. It is the purpose of this experiment to investigate the effect of this neglect on the properties of an aerosol cloud.

It may be shown [4] that the form of the particle concentration - size distribution that satisfies Equation (5) is

$$N(r, \underline{R}) = \int d^3 \underline{R}_O G(r, \underline{R} - \underline{R}_O) S(r, \underline{R}_O) \quad (8)$$

where:  $S(r, \underline{R}_O)$  = source of particles,  
 $G(r, \underline{R})$  = Green function satisfying Equation (5), and  
 $\underline{R}_O$  = coordinate of source,

if no particle growth occurs. If  $|\underline{R} - \underline{R}_O| \gg |\underline{R}_O|$ ,  $S(r, \underline{R}_O) \approx n(r) \delta(\underline{R}_O)$ , and Equation (8) becomes

$$N(r, \underline{R}) \approx n(r) G(r, \underline{R}) . \quad (9)$$

The separable approximation may then be made if there exists an average radius  $\langle r \rangle$ , such that

$$|G(\langle r \rangle, R) - \int_{r_1}^{r_2} dr G(r, R) / (r_2 - r_1)| \ll \epsilon \quad (10)$$

where  $\epsilon$  is an experimental measurement error, at arbitrarily many  $R$ . This is true when

$$\frac{dG}{dR} \ll \frac{G}{R} \quad (11)$$

where  $\tau$  is a characteristic time analogous to the collision time in classical transport theory [4]. The condition expressed by Equation (11) is commonly assumed.

In this experiment, Equation (9) is assumed; that is, a point source of particles is present. Additionally, the medium in which the diffusion occurs is assumed to be isotropic and steady state. All coordinates will be taken relative to the source streamlines. For convenience, we shall assume  $\langle r \rangle$  is given by

$$\langle r \rangle \equiv \left[ \int_{r_1}^{r_2} r^m n(r) dr \right]^{\frac{1}{m}} \quad (12)$$

where  $m$  will vary from 1 through 3. The average radius is thus a moment of the source particle size distribution function.

One of the parameters that will be examined in this experiment is the volume of particles. The volume of particles per unit volume for the differential diffusion may be calculated from Equation (9) as

$$V(R) = 4\pi/3 \int_{r_1}^{r_2} n(r) G(r, R) r^3 dr. \quad (13)$$

The volumes corresponding to average radii, called herein the average volume, are

$$\langle V \rangle = 4\pi/3 G(\langle r \rangle, R) \int_{r_1}^{r_2} n(r) r^3 dr. \quad (14)$$

The calculation of Equation (13) will be further discussed in the next section.

### III. OPTICAL PROPERTIES

In the previous section, the extinction coefficient was given as

$$\alpha(\underline{R}) \approx \int_{r_1}^{r_2} N(r, \underline{R}) \sigma(r) dr \quad (3)$$

which may be rewritten in the form

$$\alpha(\underline{R}) \approx \int_{r_1}^{r_2} n(r) G(r, \underline{R}) \sigma(r) dr \quad (15)$$

by substitution of Equation (9). We now introduce the approximation that

$$|G(r + \delta r, \underline{R}) - G(r, \underline{R})| \ll \epsilon \quad (16)$$

and that

$$|\sigma(r + \delta r) - \sigma(r)| \ll \pi r^2, \quad (17)$$

for suitably small  $\delta r$ . This approximation allows  $\alpha(\underline{R})$  to be further approximated as

$$\alpha(\underline{R}) \approx \sum_{n=1}^N \pi Q(r_n) G(r_n, \underline{R}) \int_{r_n}^{r_n + \delta r} r^2 n(r) dr \quad (18)$$

where:  $\delta r = (r_2 - r_1) / (N-1)$ , and

$Q$  = Mie scattering efficiency factor<sup>2</sup>.

Another parameter that will be examined is optical depth, the integral of the extinction coefficient along a line-of-sight. The total optical depth can be calculated from Equation (19) as

$$\tau \approx \pi \sum_n Q(r_n) \left\{ \int_{-\infty}^{+\infty} G(r_n, R) dx \right\} \left\{ \int_{r_n}^{r_n + \delta_r} r^2 n(r) dr \right\} \quad (19)$$

The last parameter to be examined is the transmission, which is given by the Beer-Lambert-Bouger Law if scattering is neglected,

$$T \approx \exp(-\tau). \quad (20)$$

Within this same approximation, other previously defined quantities may be approximated. The volume of particles, Equation (13), may be rewritten as

$$V(R) \approx 4\pi/3 \sum_n G(r_n, R) \int_{r_n}^{r_n + \delta_r} r^3 n(r) dr. \quad (21)$$

The average optical depth and average transmission corresponding to the average radii are

$$\langle \tau \rangle \approx \alpha \int_{-\infty}^{+\infty} G(\langle r \rangle, R) dx, \quad (22)$$

and

$$\langle T \rangle = \exp(-\langle \tau \rangle),$$

respectively.

It should be noted that the terms called averages are not truly averages over the cloud. Rather they refer only to the average radii.

#### IV. EXPERIMENTAL

In this section, the use of the equations developed in Sections II and III will be discussed. Nine excursions will be described. The particle size distribution function  $n(r)$  and the moment  $m$  will be varied. Three size distribution functions will be used, two Junge distributions [5], given by

$$n(r) = Ar^{-4} \quad (23)$$

and

$$n(r) = Br^{-3} \quad (24)$$

where: A and B = constants, and a Deirmendjian distribution [2] given by

$$n(r) = a r^{\gamma} \exp(-br) \quad (25)$$

where: a,  $\gamma$ , and b are constants. The parameters are adjusted to give the same total number of particles and for the Deirmendjian distribution to lie approximately between the two Junge distributions for large r.

Three moments ( $m = 1, 2$ , and 3) were used corresponding to the radius, the area, and the volume moment. Calculations were then performed using these particle size distributions of the volume of particles, the extinction coefficient, the optical depth, and the transmission. The results of these calculations are shown in *Figures 1 through 81*.

The curves of volume are given in *Figures 1 through 12*. In all cases, the volume of particles predicted by the average diffusion parametrization is less and more sharply contained than that predicted by the exact formalism. If an average diffusion parametrization were used to analyze experimental data, excessively large diffusion coefficients would be required. Exactly similar behavior is also demonstrated by the extinction coefficient, *Figures 13 through 24*, and by optical depth, *Figures 25 through 36*.

The surprise in the experiment may be found in the transmission, *Figures 37 through 81*. Large differences may be seen in the transmission curves of the Junge distributions, *Figures 37 through 66*, although the clouds are sharp. In the transmission of the Deirmendjian haze, however, surprisingly good agreement may be seen. Further, the degree of agreement does not appear to vary strongly with moment. This is probably due to the fact that the moments of this distribution do not vary rapidly with change in moment. Additionally, it is heartening since this distribution is most similar to the log normal distribution normally used in modeling smoke.

## V. CONCLUSIONS

The volume of particles, extinction coefficient, optical depth, and transmission for aerosol clouds were calculated using both particle size averaged and size dependent diffusion. Non-diffusive contributions to the particle size distributions were not considered. Large differences between the average and exact calculations were evidenced for all calculations and particle size distributions except for transmission through a Deirmendjian haze distribution.

The results of this experiment do yield some insight into the utility of the average diffusion approximation commonly used in smoke modeling. These models should be acceptably accurate for simulation of transmission, but possibly not for simulation of concentration. By the same token, these models should be validated against transmission measurements and not against concentration measurements. Additionally, selection of an average particle size distribution is critical.

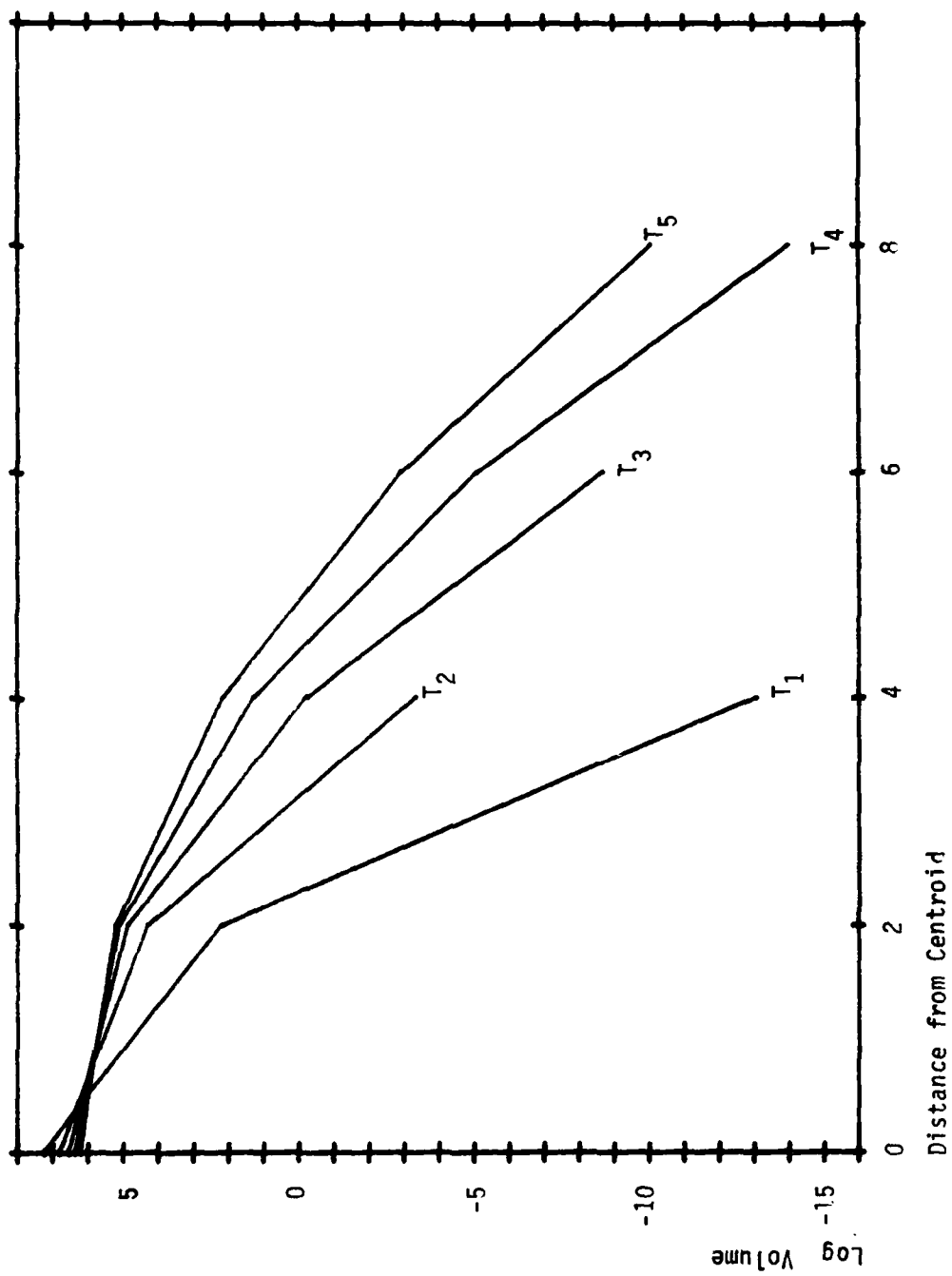


Figure 1. Average volume versus distance, first moment average,  $n(r) = 1/r^4$ .

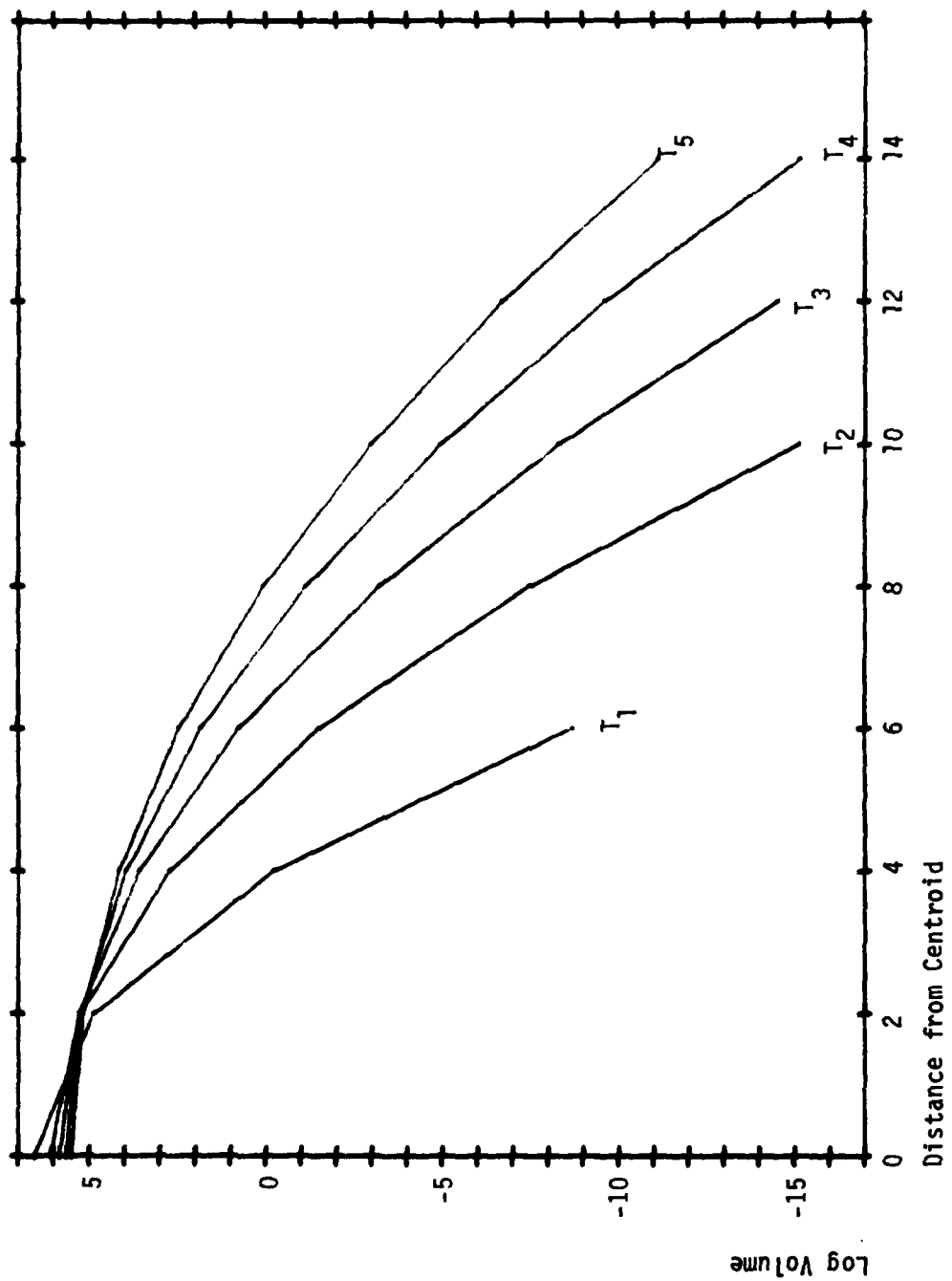


Figure 2. Average volume versus distance, second moment average,  $n(r) = 1/r$ .

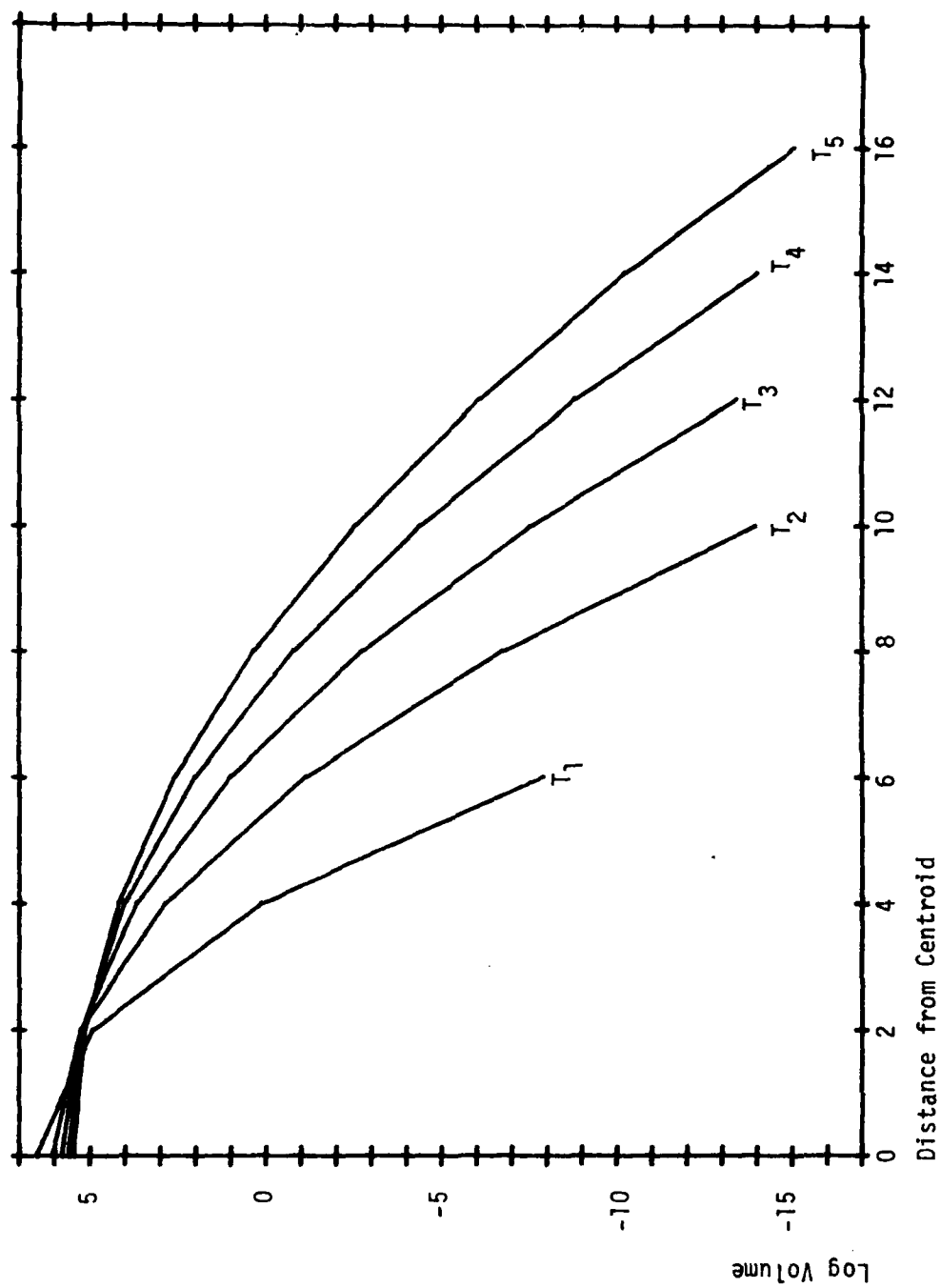


Figure 3. Average volume versus distance, third moment average,  $n(r) = 1/r^4$ .

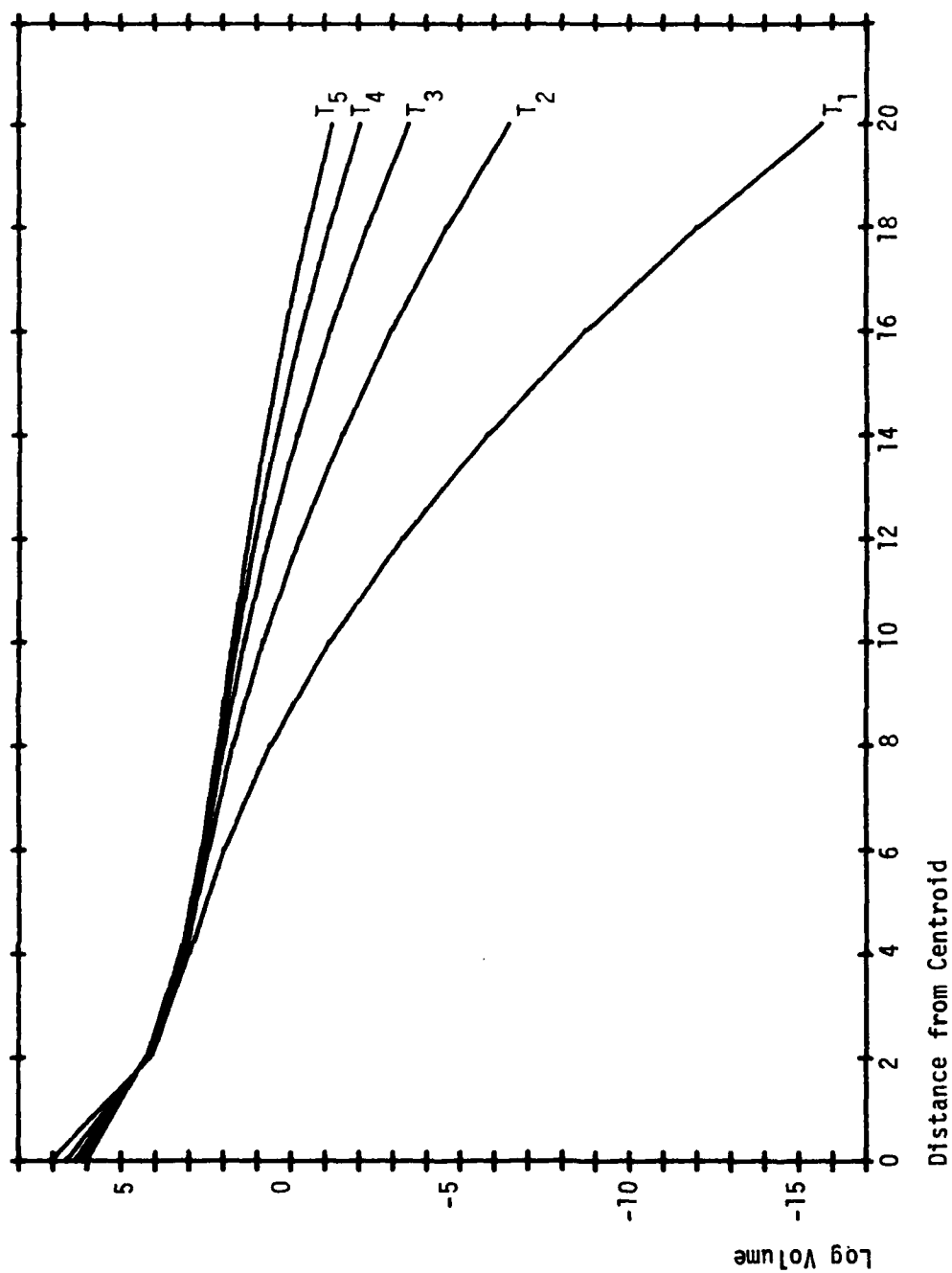


Figure 4. Volume versus distance,  $n(r) = 1/r^4$ .

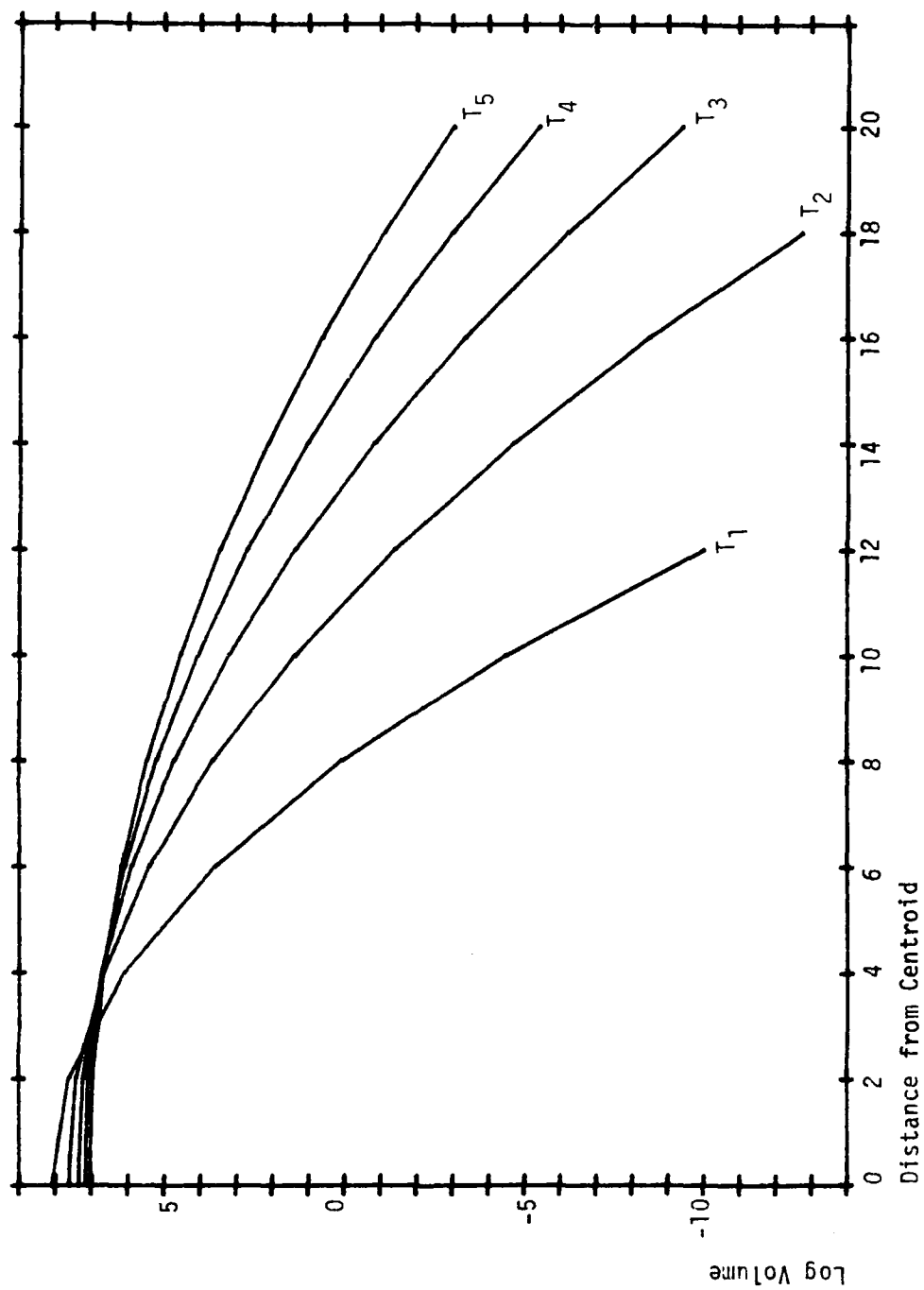


Figure 5. Average volume versus distance, first moment average,  $n(r) = 1/r^3$ .

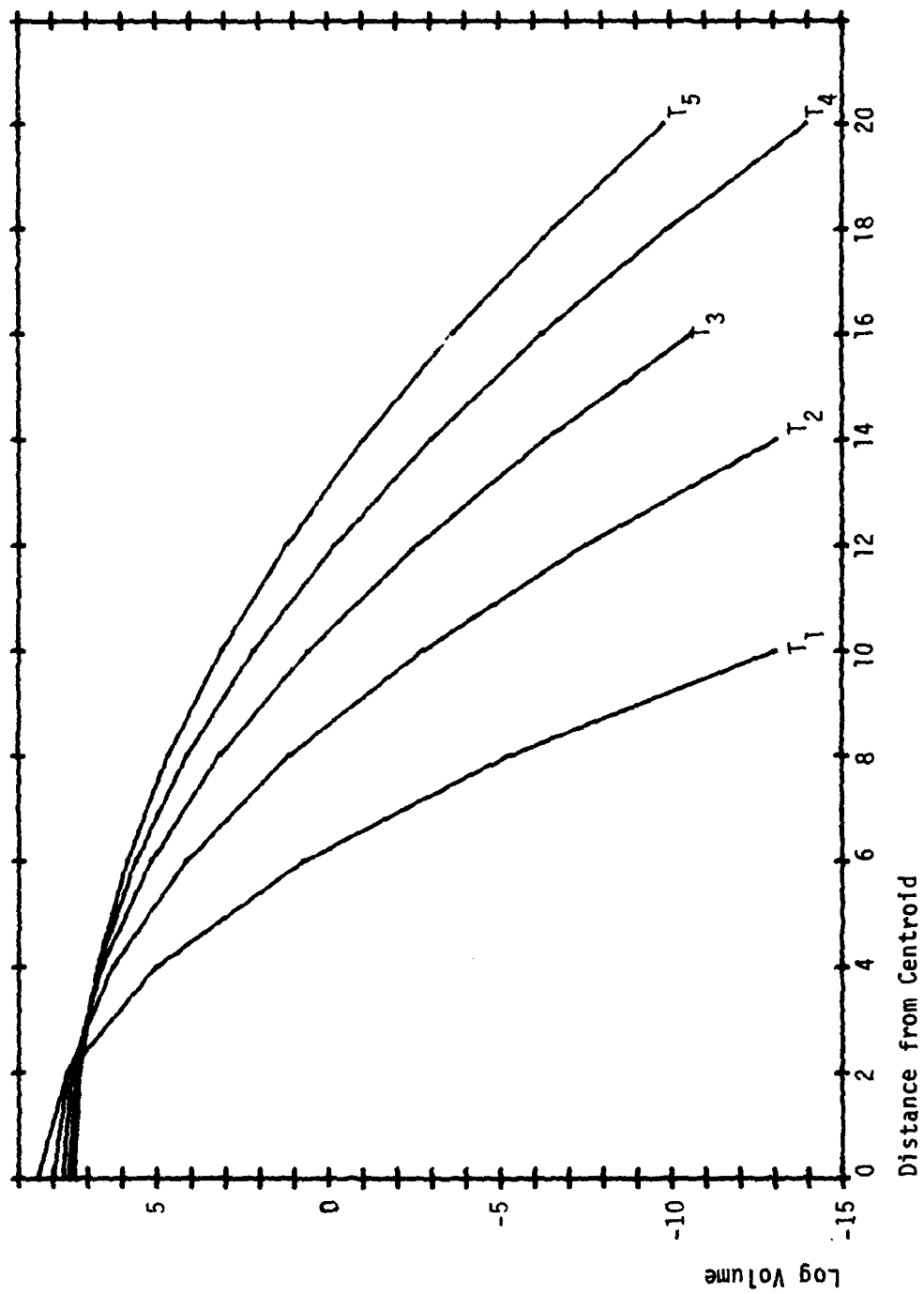


Figure 6. Average volume versus distance, second moment average,  $n(r) = 1/r^2$ .

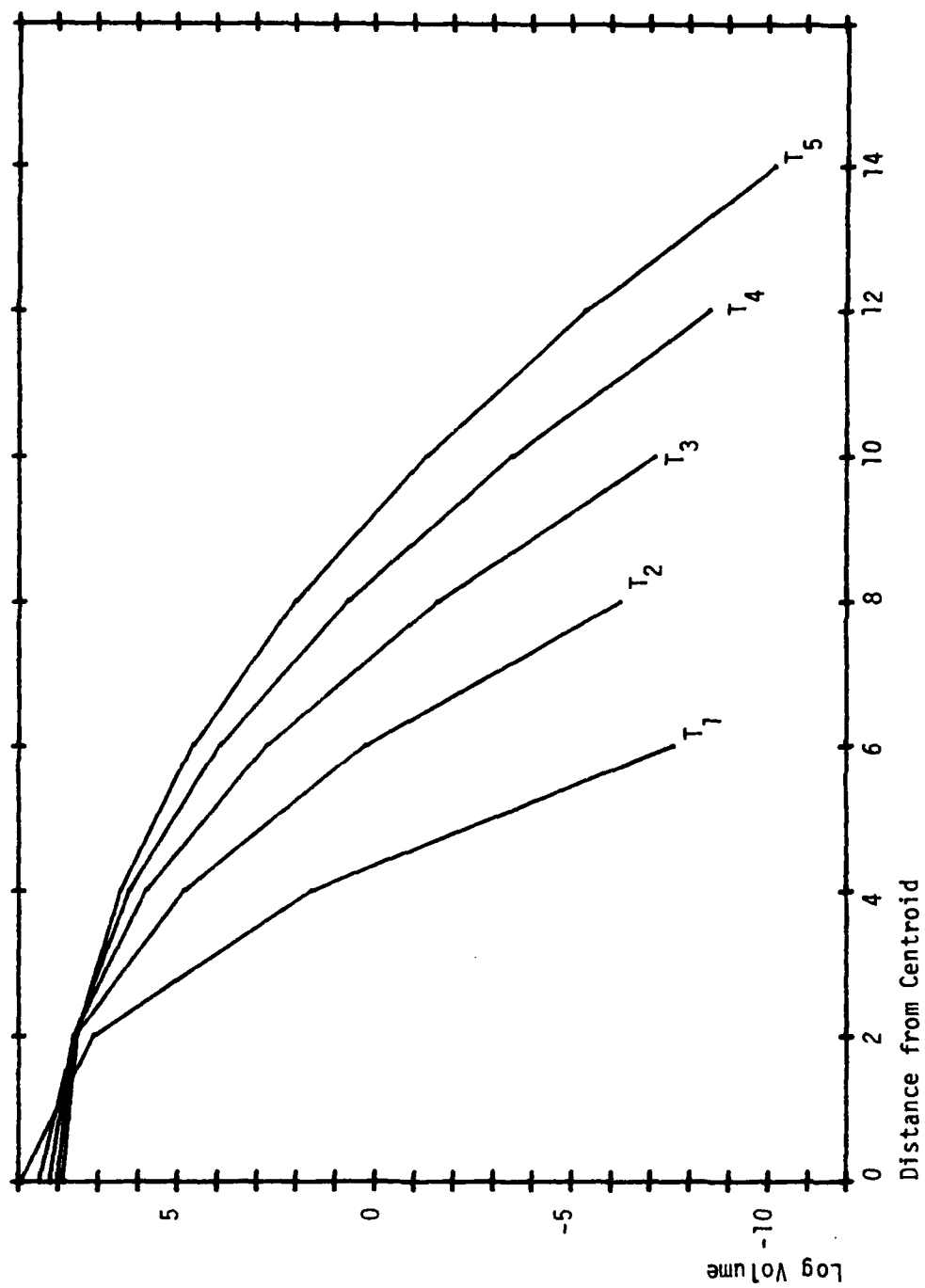


Figure 7. Average volume versus distance, third moment average,  $n(r) = 1/r^3$ .

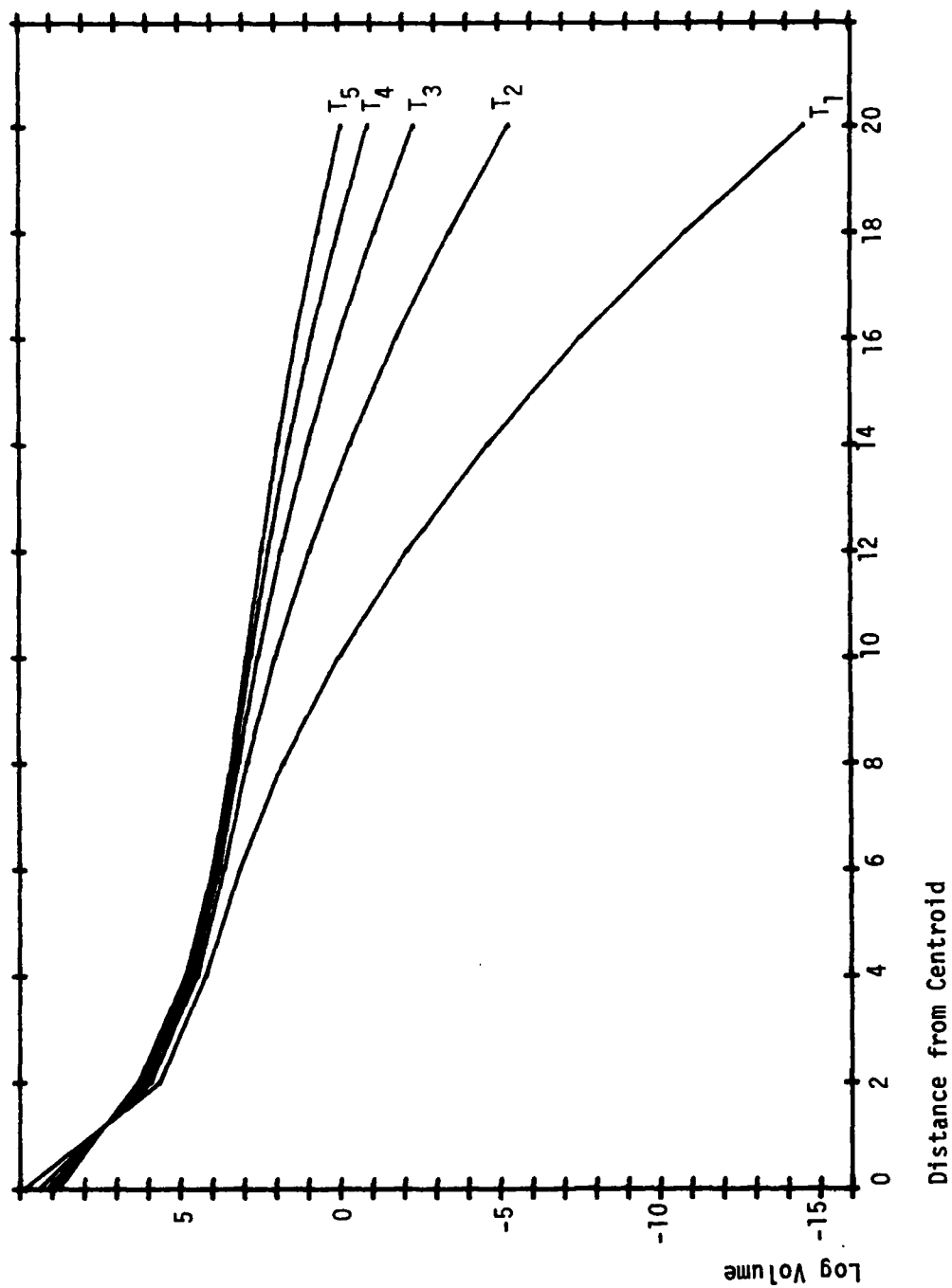


Figure 8. Volume versus distance,  $n(r) = 1/r^3$ .

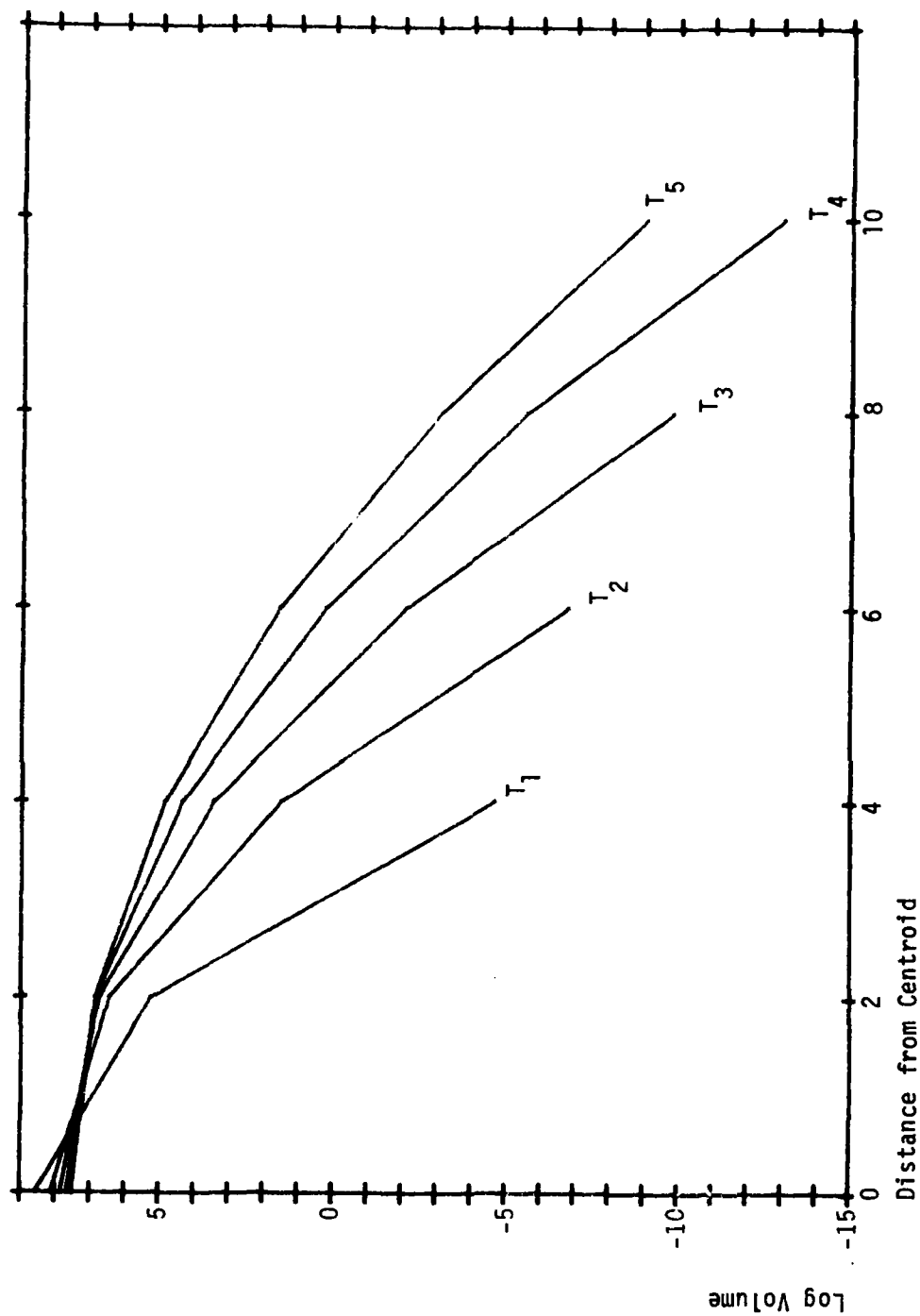


Figure 9. Average volume versus distance, first moment average,  
 $n(r)$  = Deirmendjian haze H.

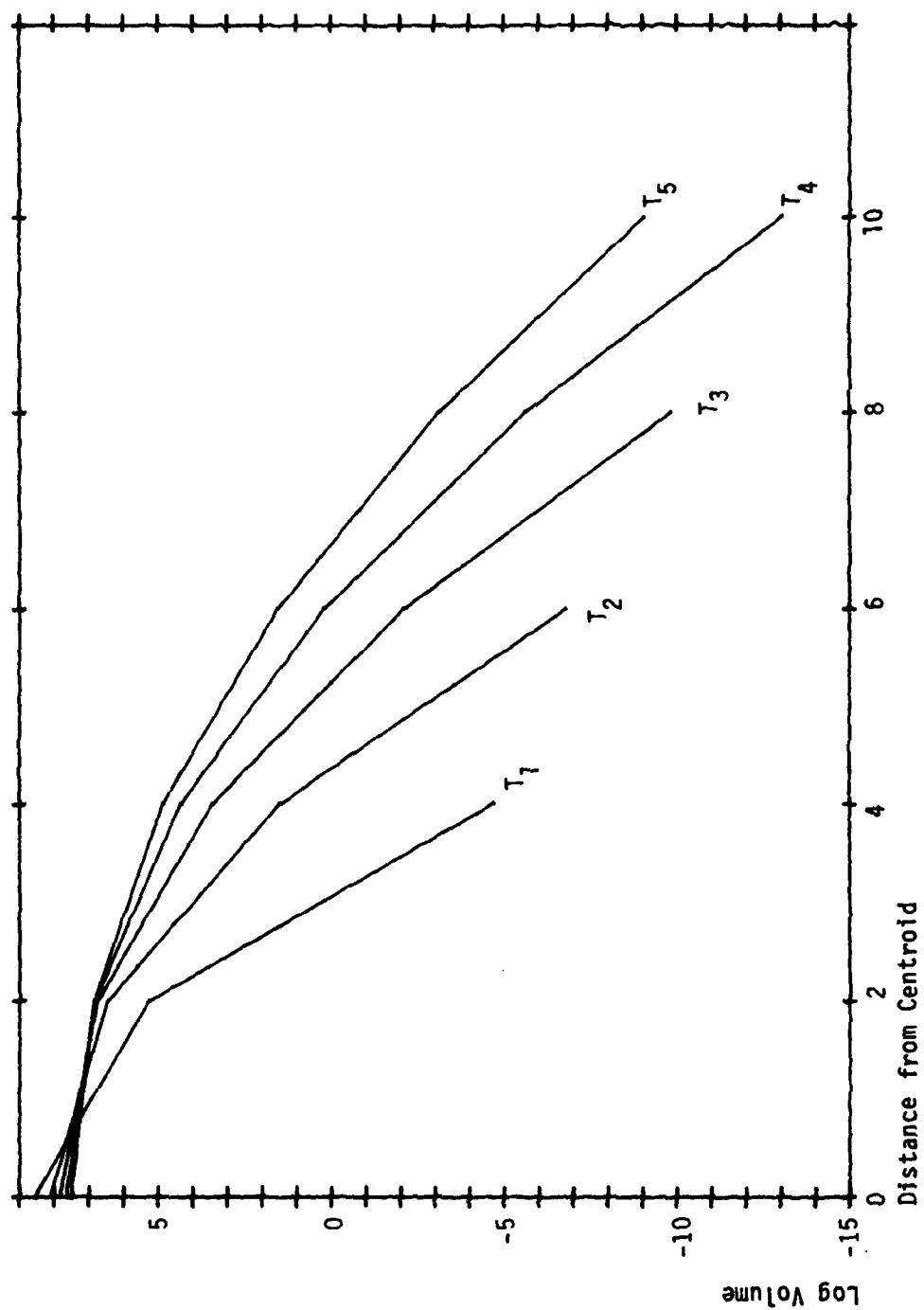


Figure 10. Average volume versus distance, second moment average,  
 $n(r)$  = Deirmendjian haze H.

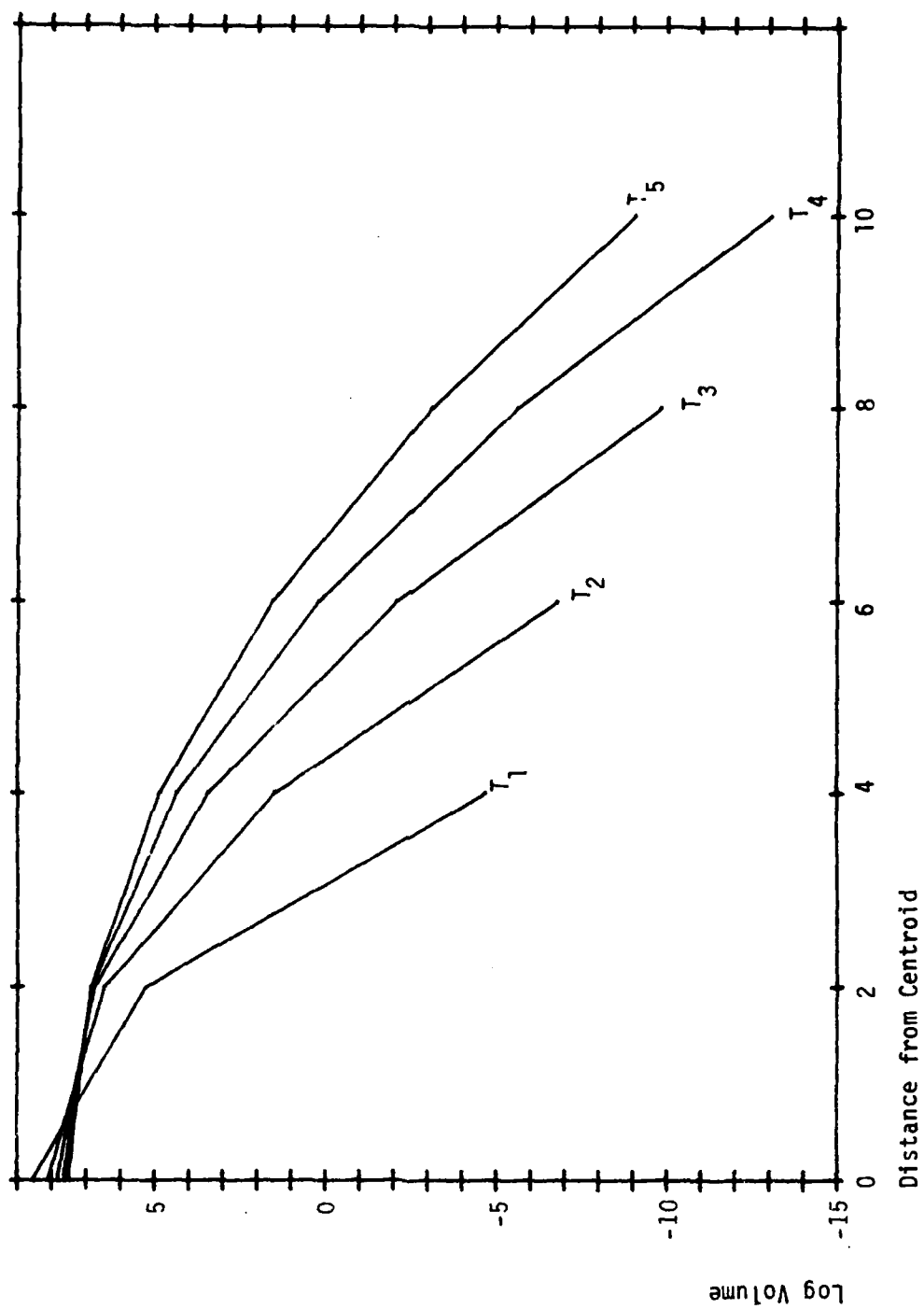


Figure 11. Average volume versus distance, third moment average,  
 $n(r) = \text{Deirmendjian haze } H.$

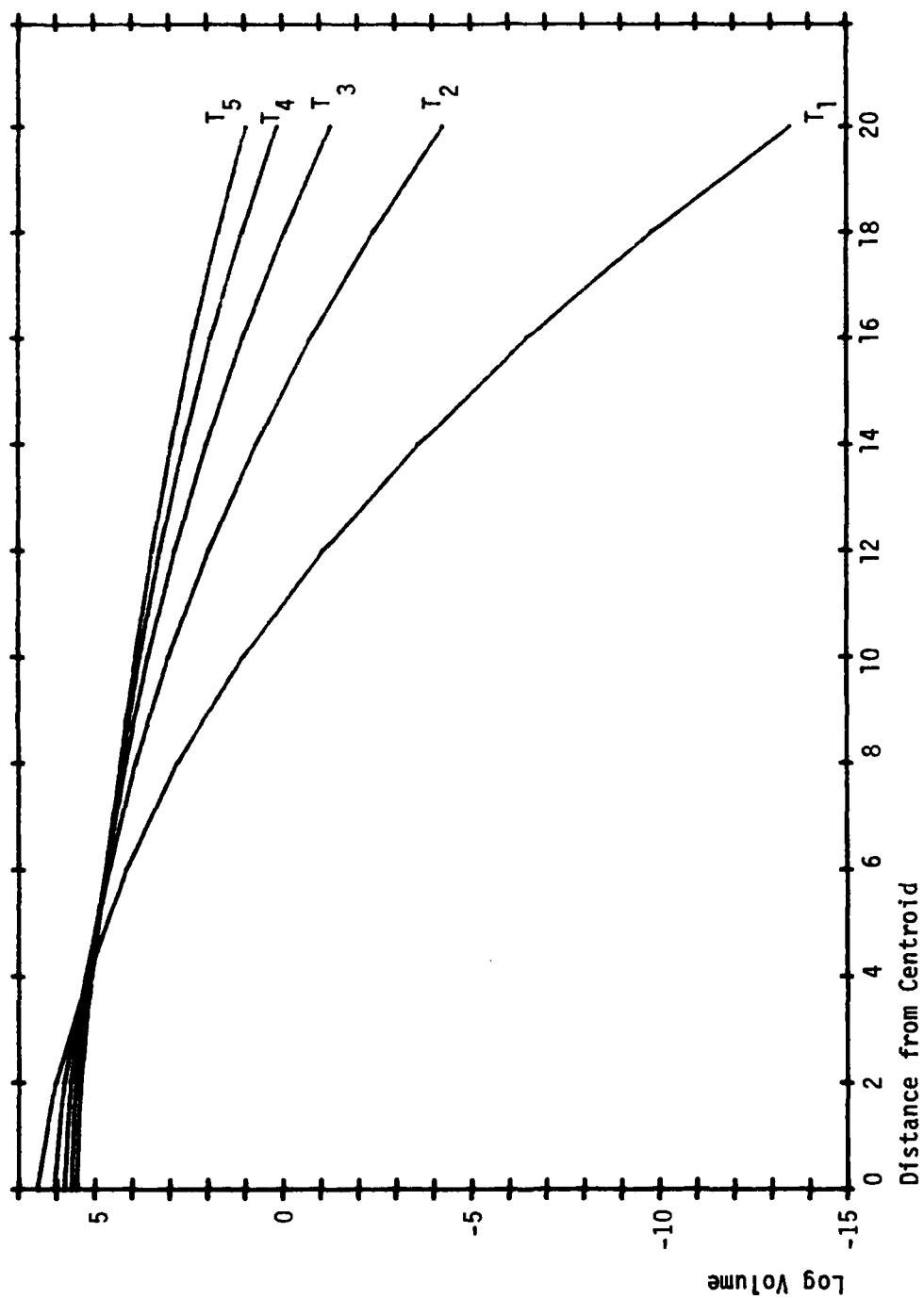


Figure 12. Volume versus distance,  $n(r)$  = Deirmendjian haze H.

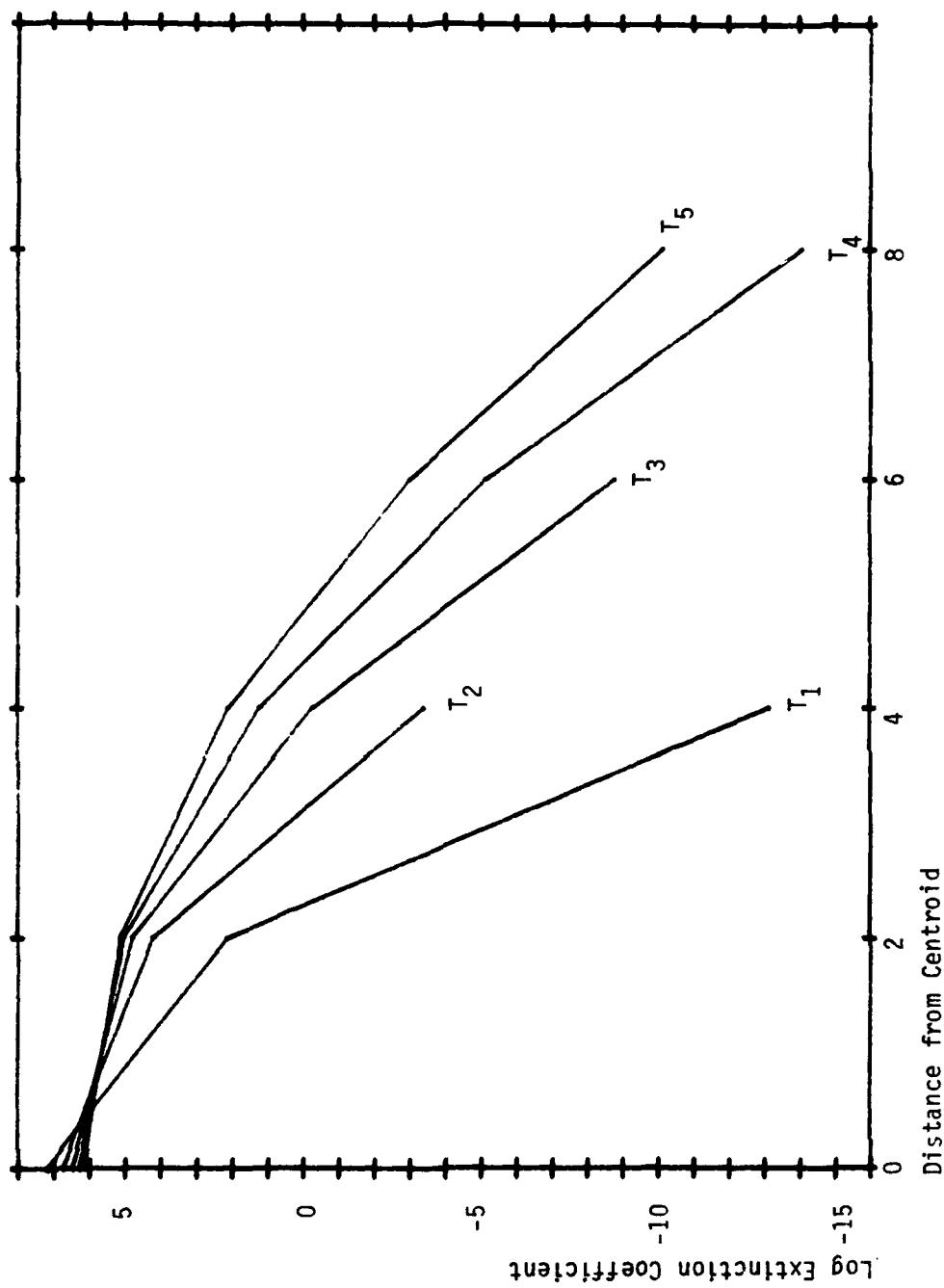


Figure 13. Average extinction coefficient versus distance, first moment average,  
 $n(r) = 1/r^4$ .

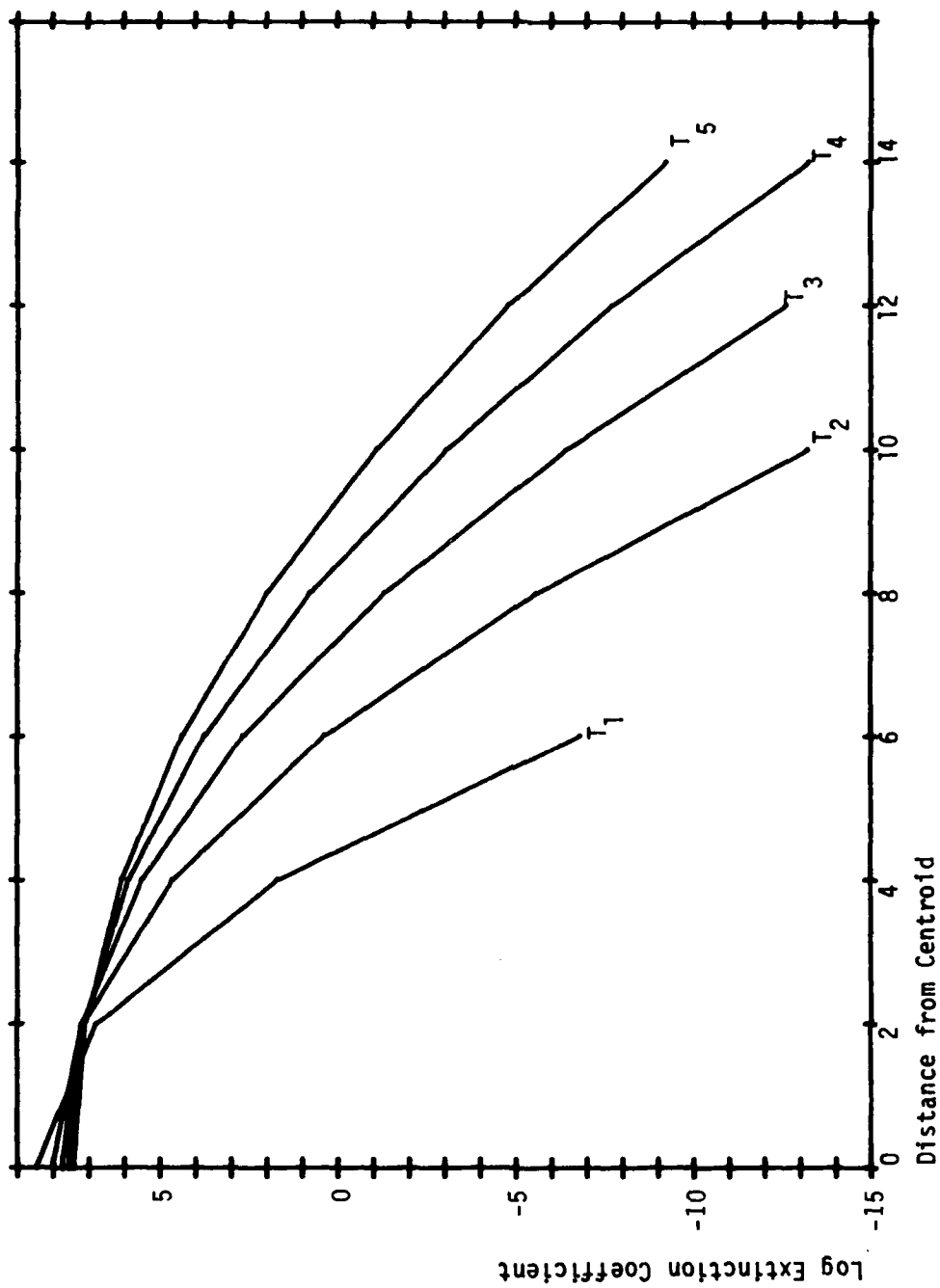


Figure 14. Average extinction coefficient versus distance, second moment average,  
 $n(r) = 1/r^4$ .

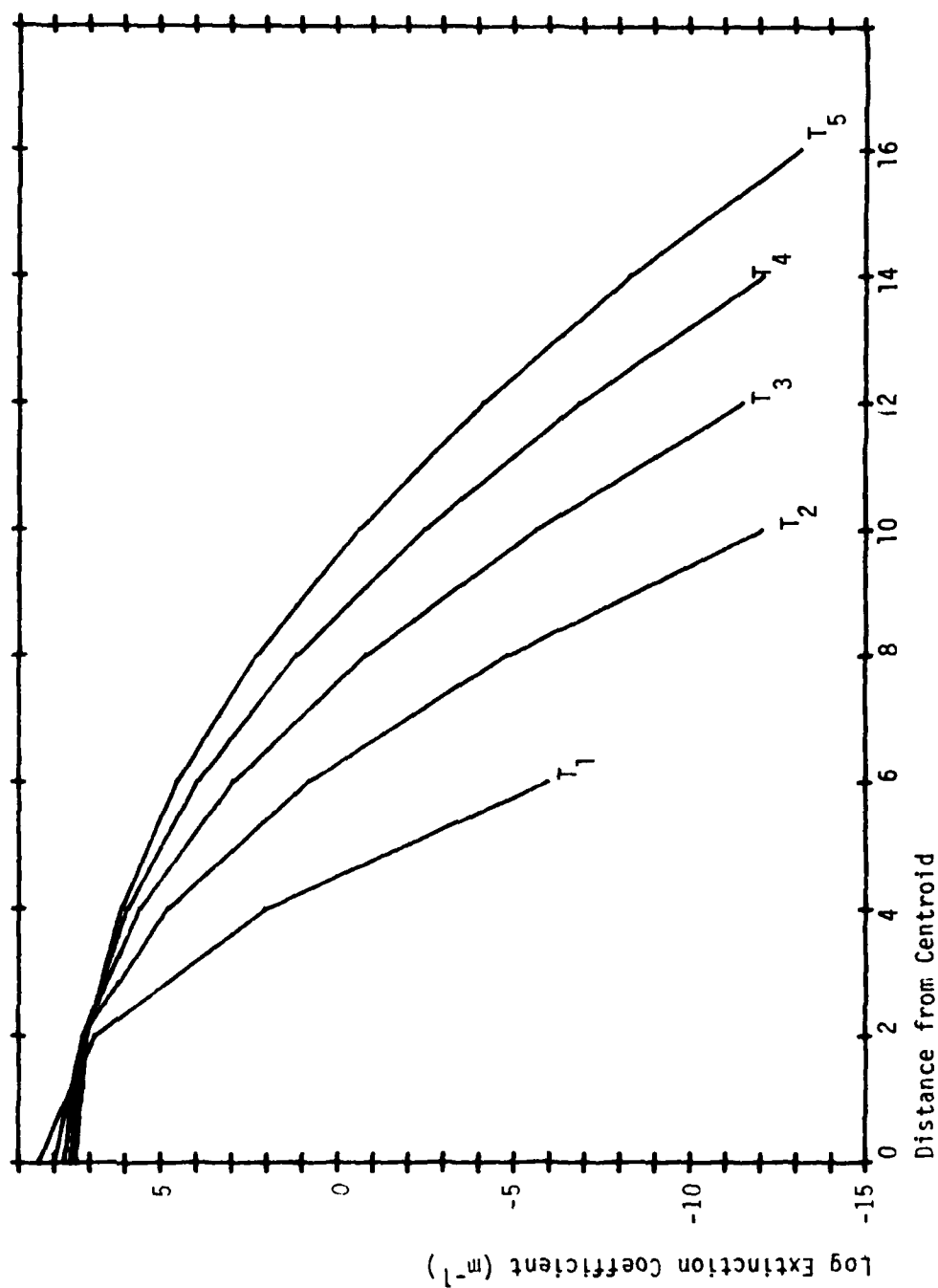


Figure 15. Average extinction coefficient versus distance, third moment average,  $n(r) = 1/r^4$ .

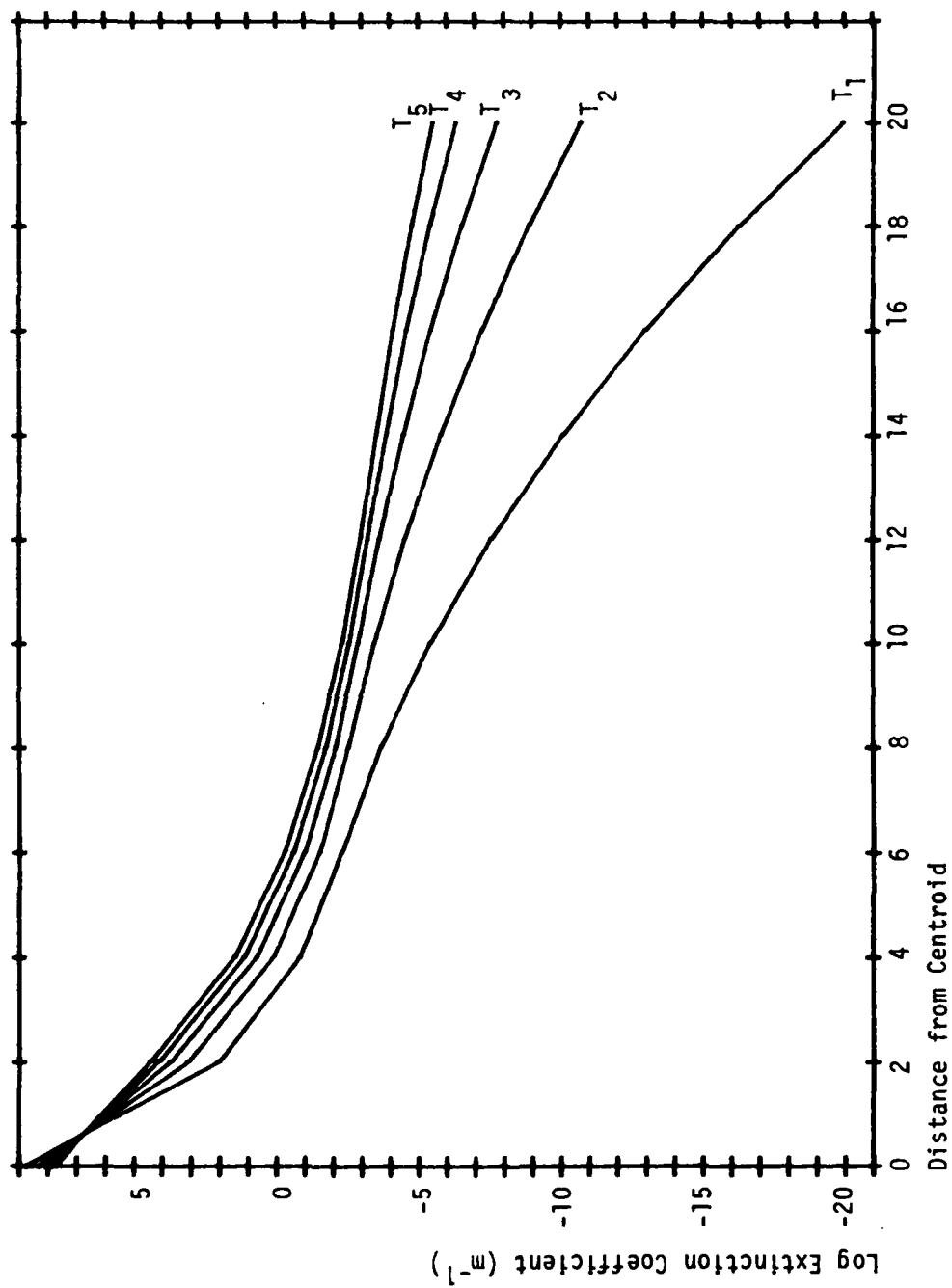


Figure 16. Extinction coefficient versus distance,  $n(r) = 1/r^4$ .

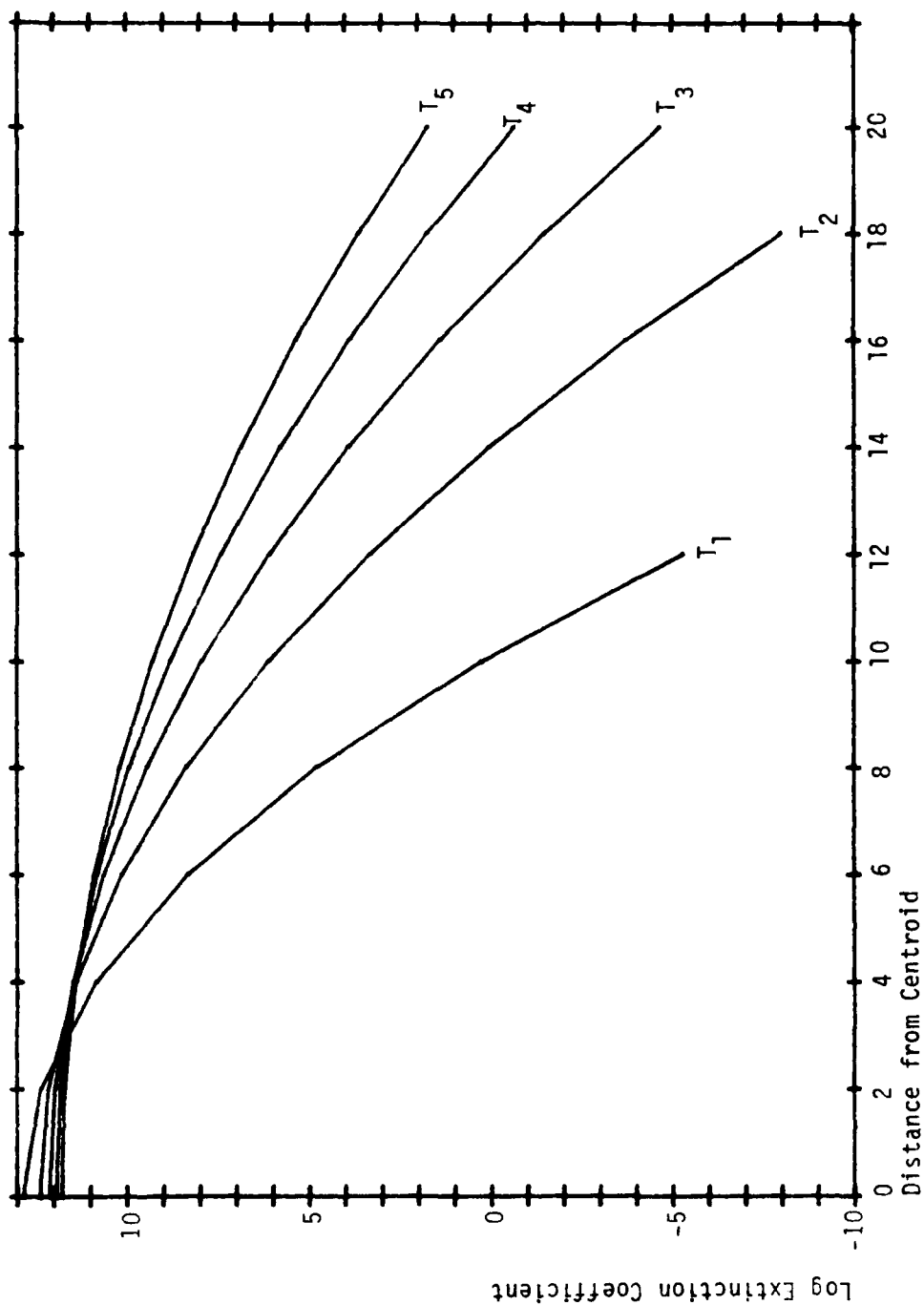


Figure 17. Average extinction coefficient versus distance, first moment average,  
 $n(r) = 1/r^3$ .

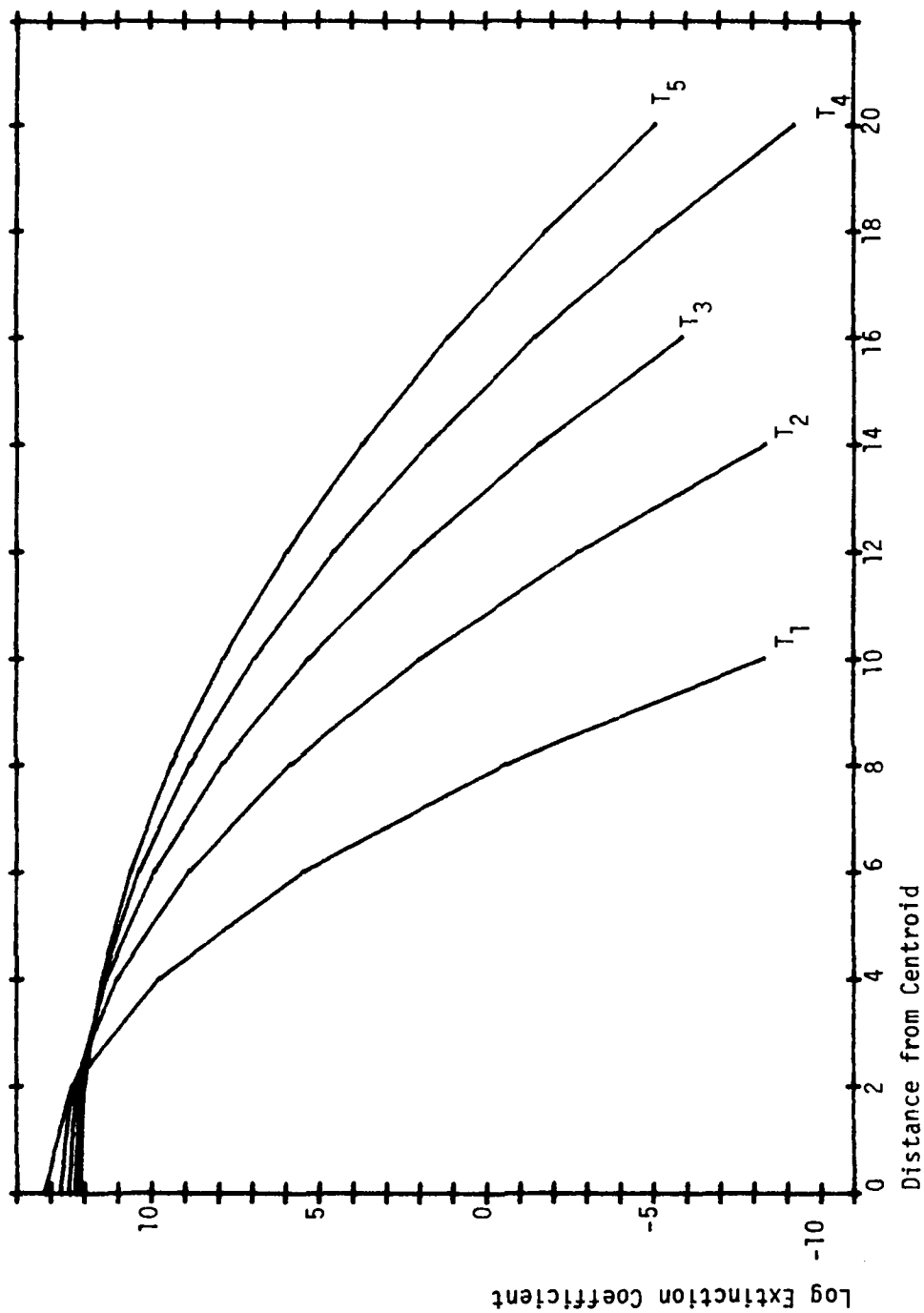


Figure 18. Average extinction coefficient versus distance, second moment average,  
 $n(r) = 1/r^3$ .

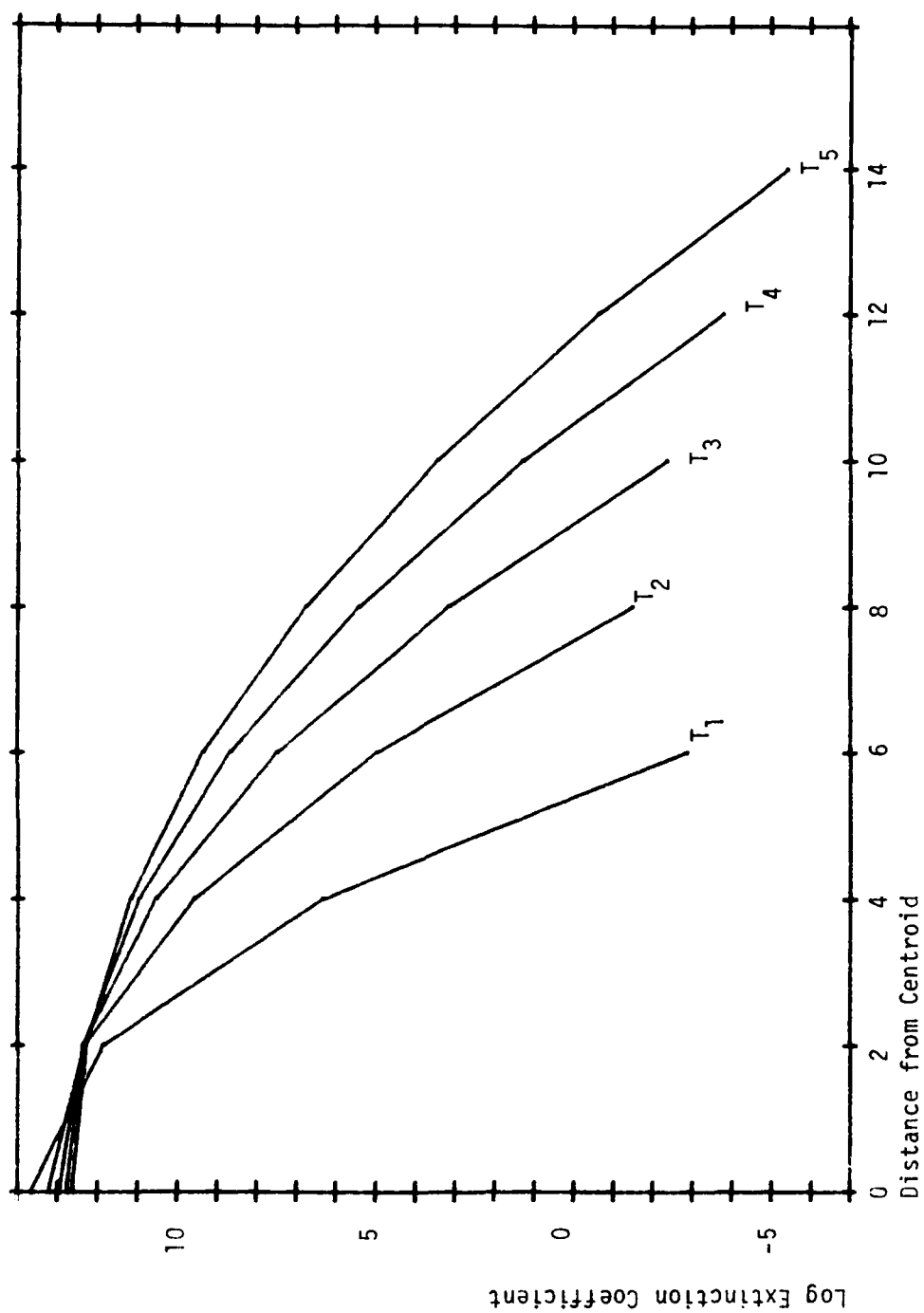


Figure 19. Average extinction coefficient versus distance, third moment average,  
 $n(r) = 1/r^3$ .

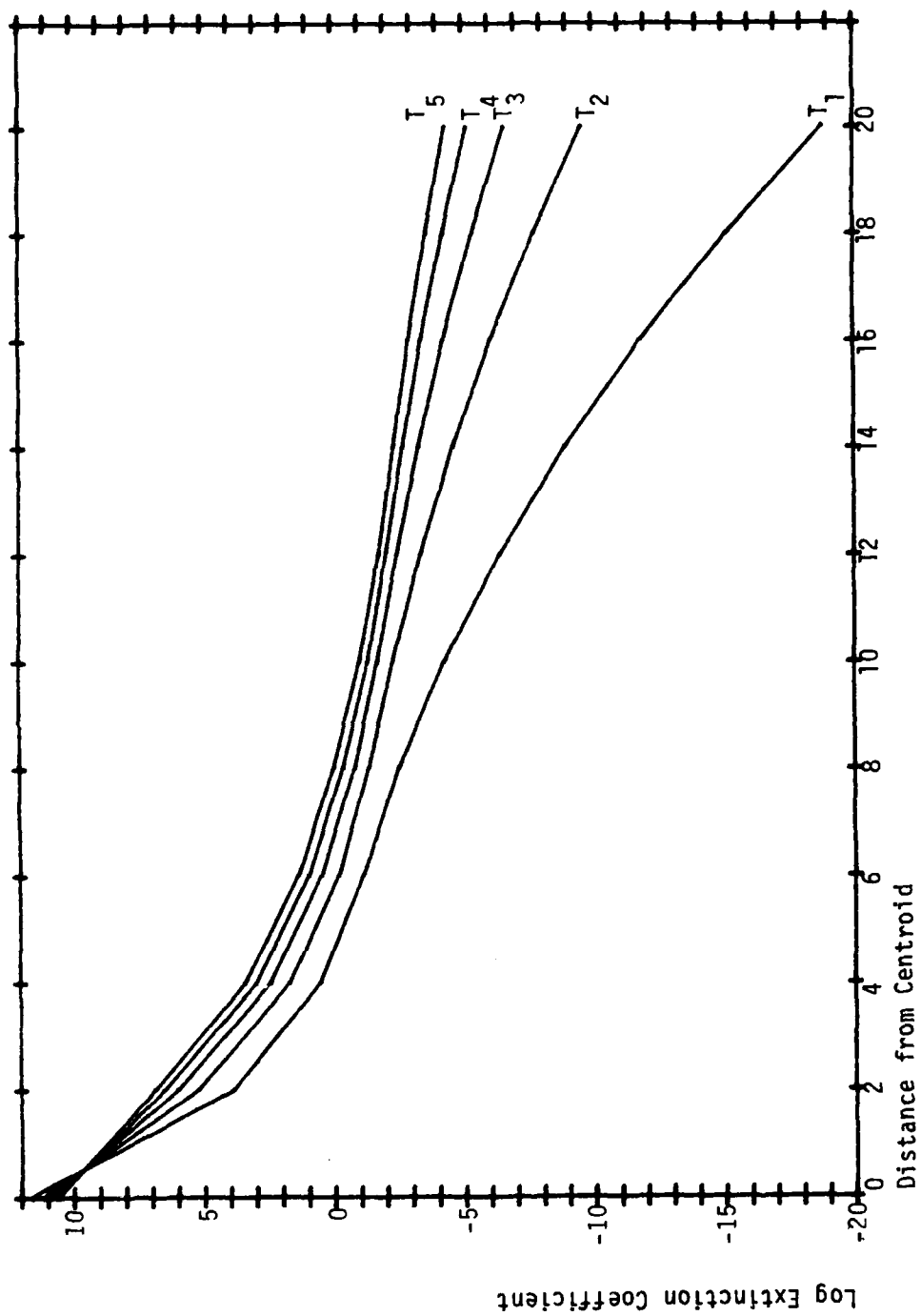


Figure 20. Extinction coefficient versus distance,  $n(r) = 1/r^2$ .

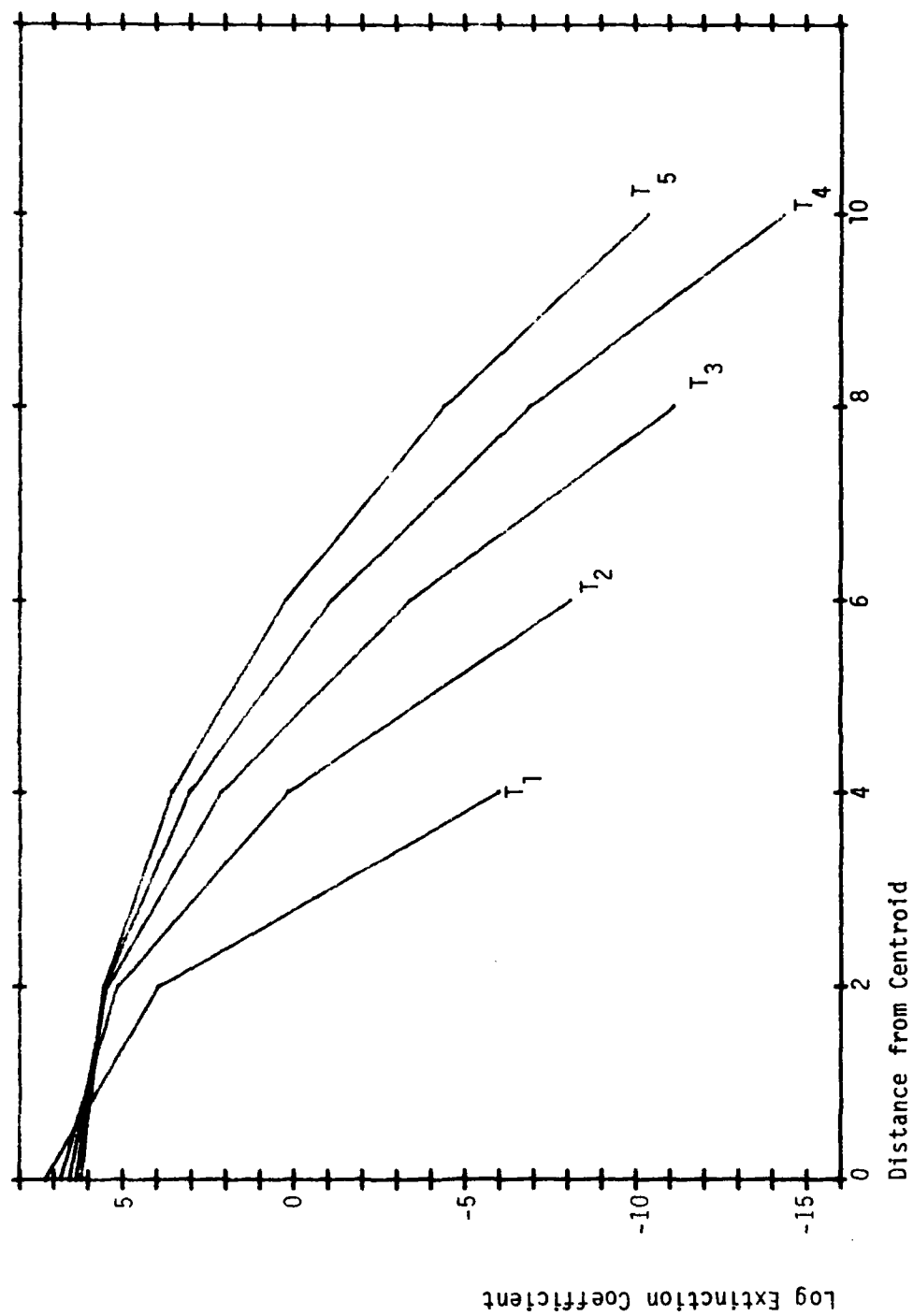


Figure 21. Average extinction coefficient versus distance, first moment average,  
 $n(r)$  = Deirmendjian haze H.

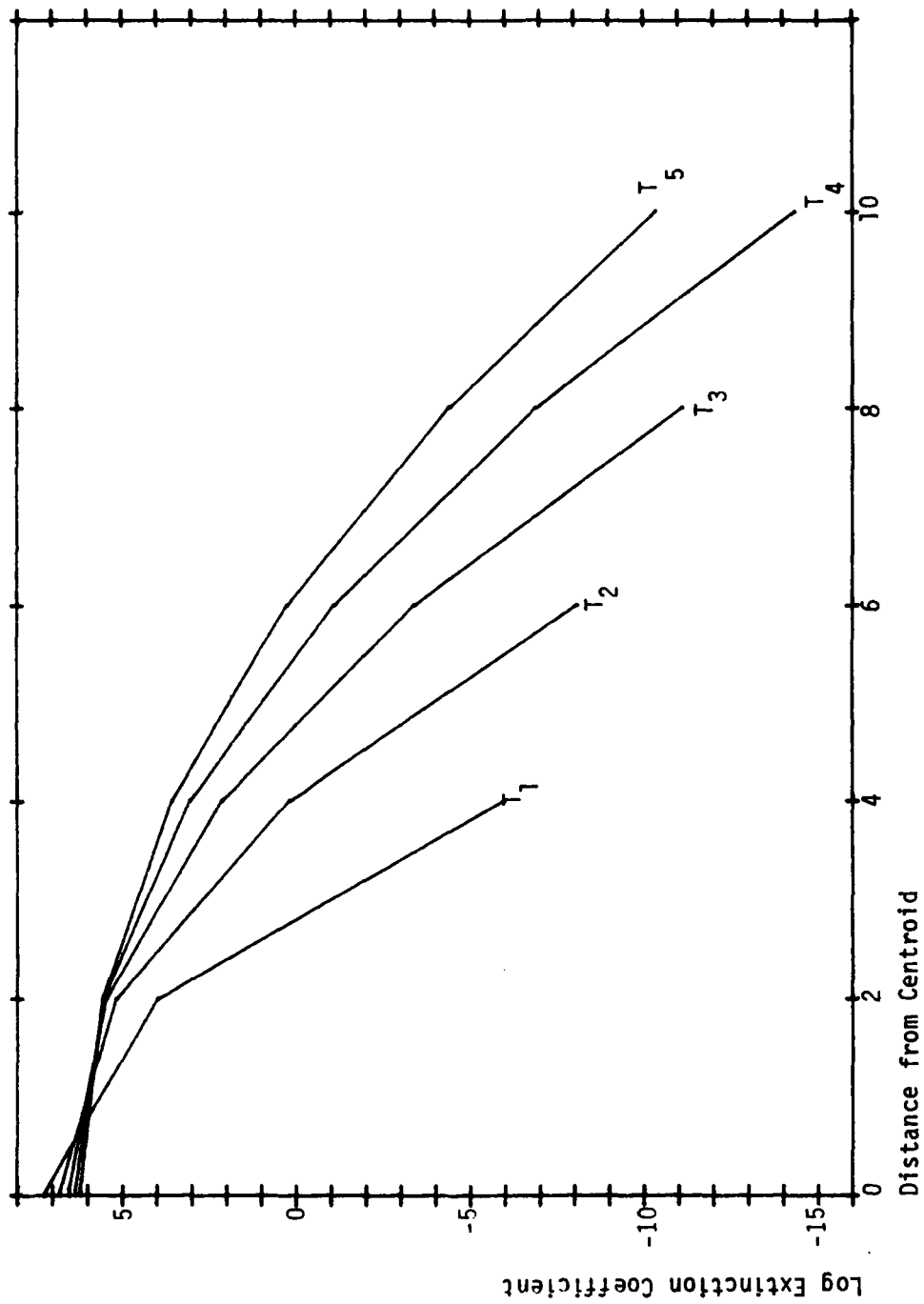


Figure 22. Average extinction coefficient versus distance, second moment average,  
 $n(r)$  = Deirmendjian haze H.

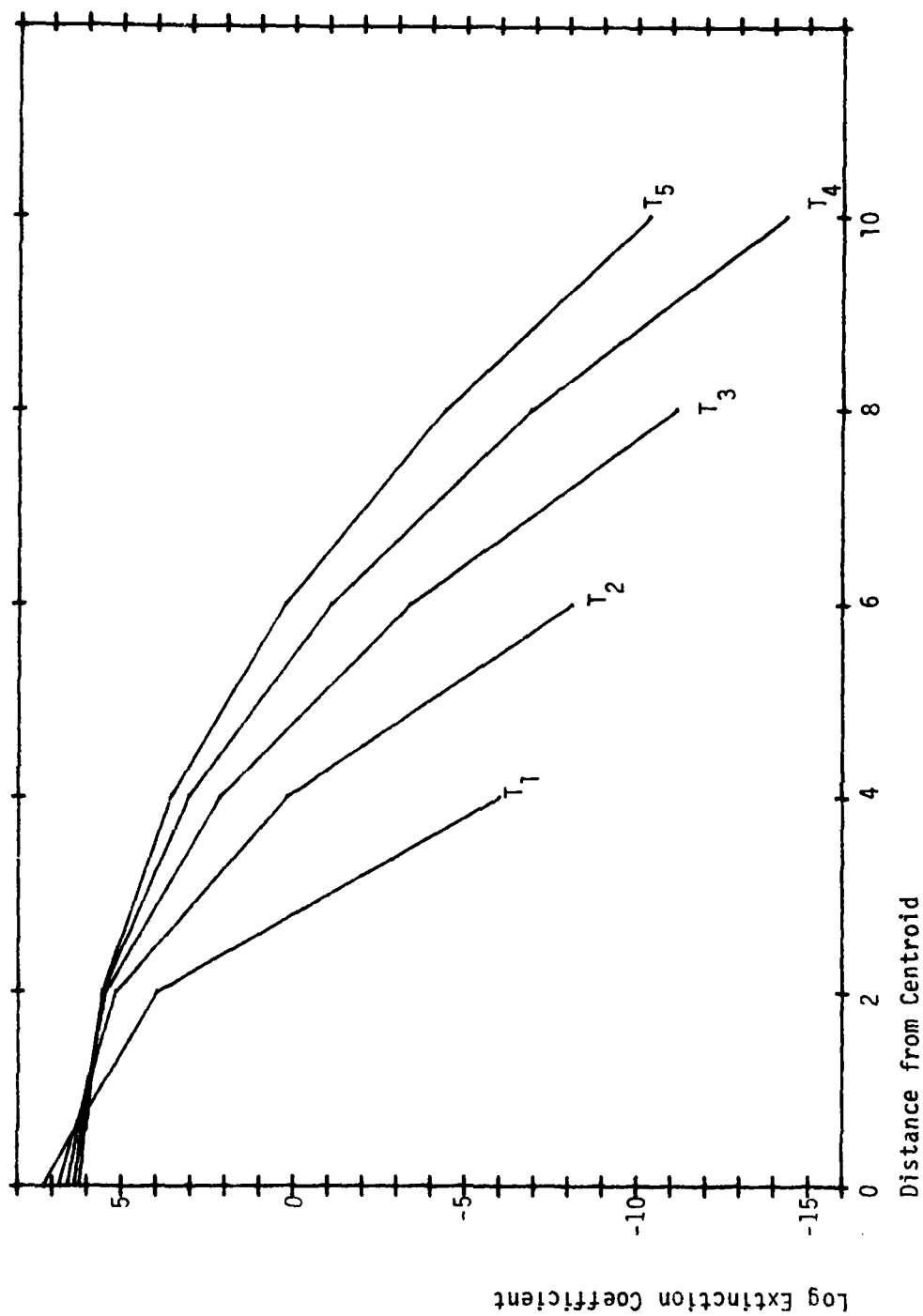


Figure 23. Average extinction coefficient versus distance, third moment average,  
 $n(r)$  = Deirmendjian haze H.

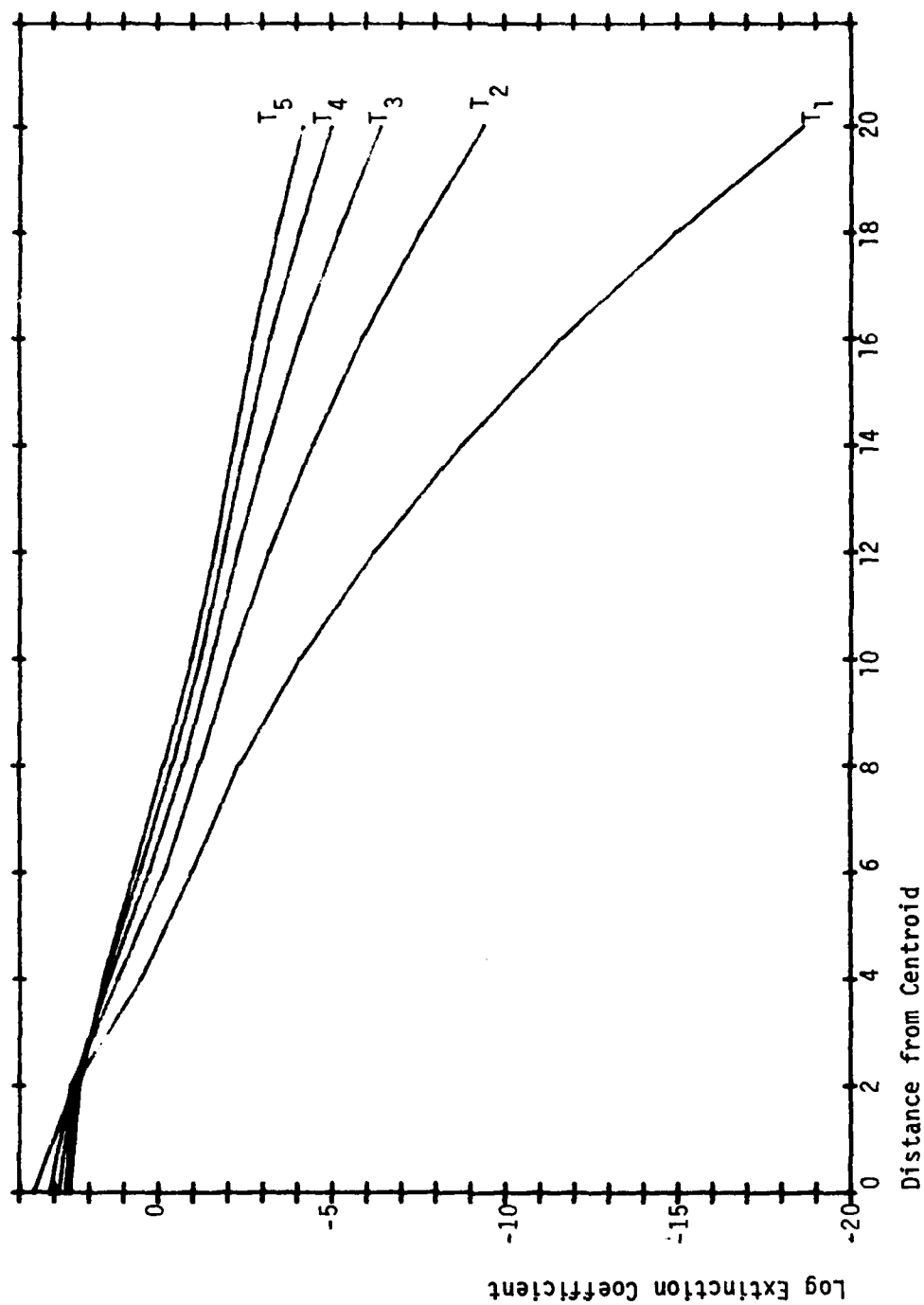


Figure 24. Extinction coefficient versus distance,  $n(r)$  = Deirmendjian haze H.

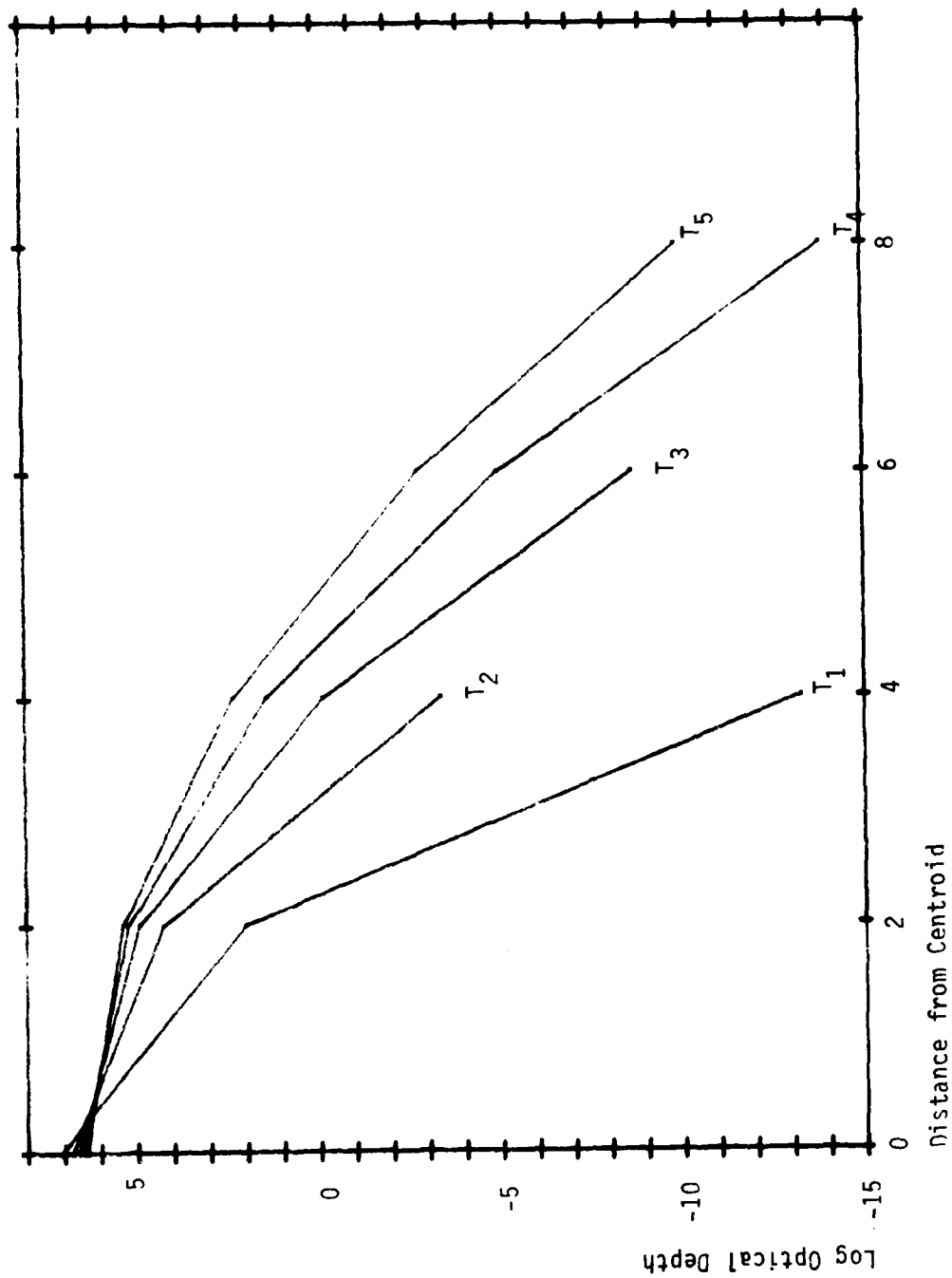


Figure 25. Average optical depth versus distance, first moment average,  
 $n(r) = 1/r^4$ .

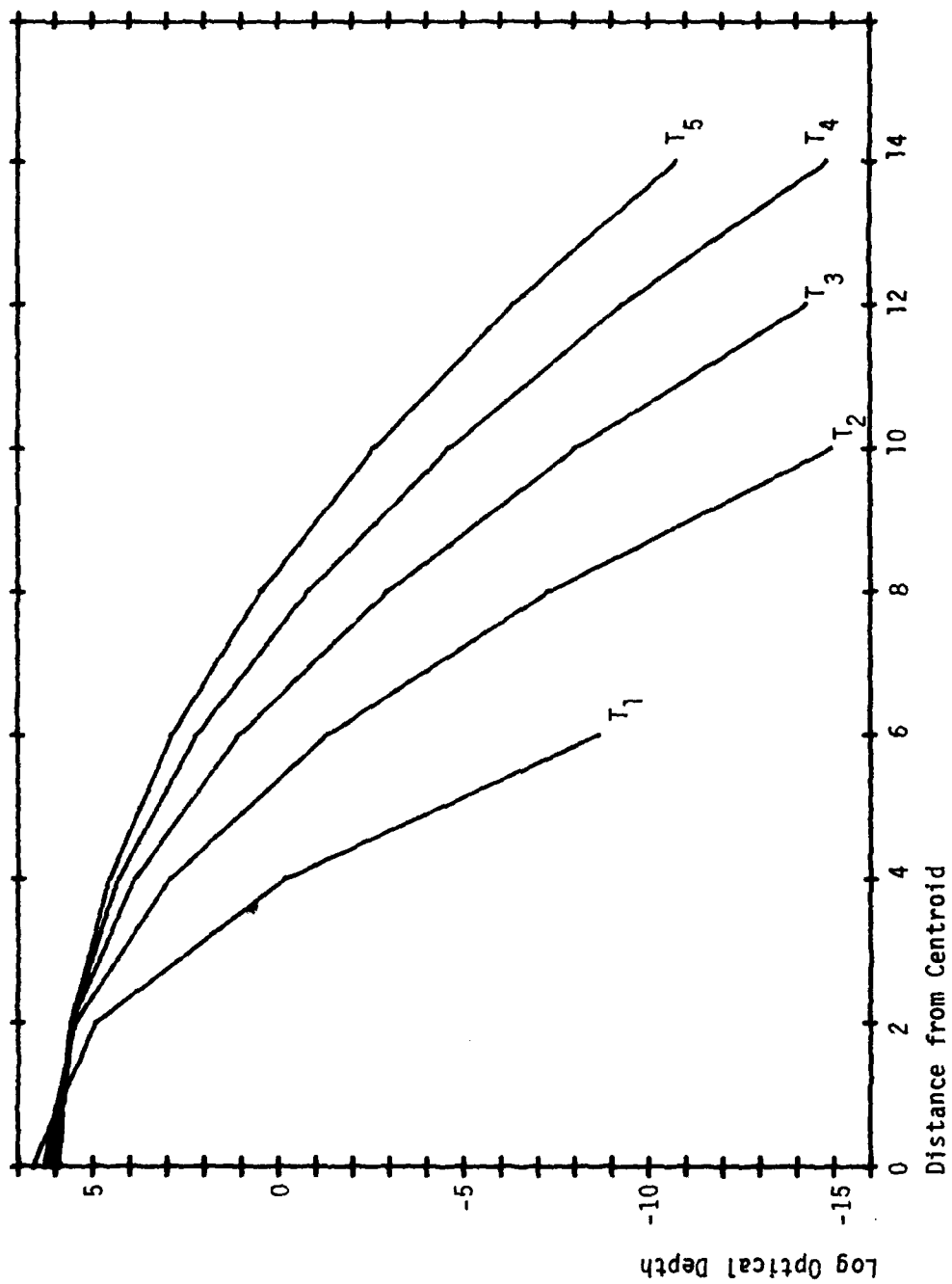


Figure 26. Average optical depth versus distance, second moment average,  
 $n(r) = 1/r^4$ .

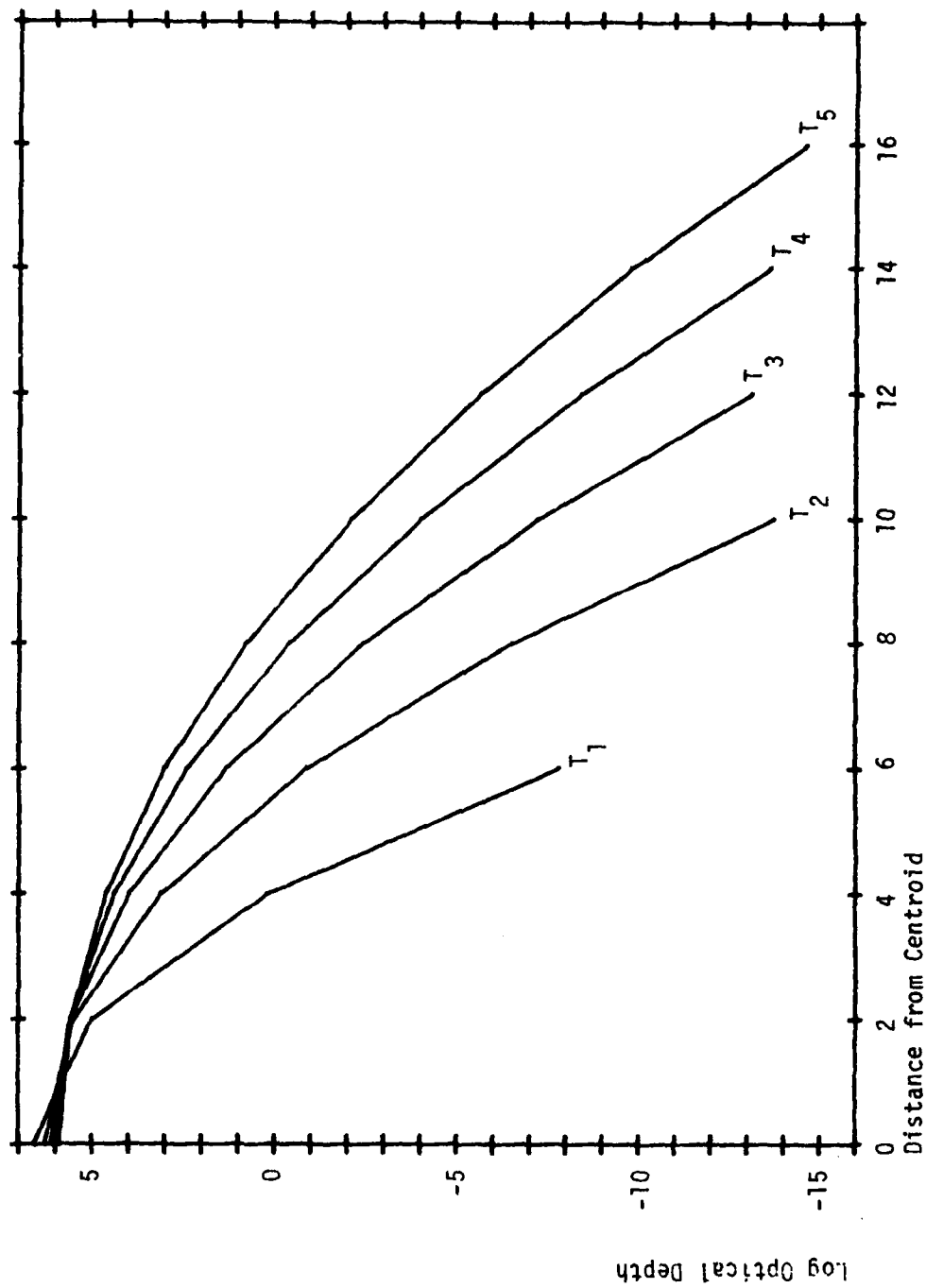


Figure 27. Average optical depth versus distance, third moment average,  
 $n(r) = 1/r^4$ .

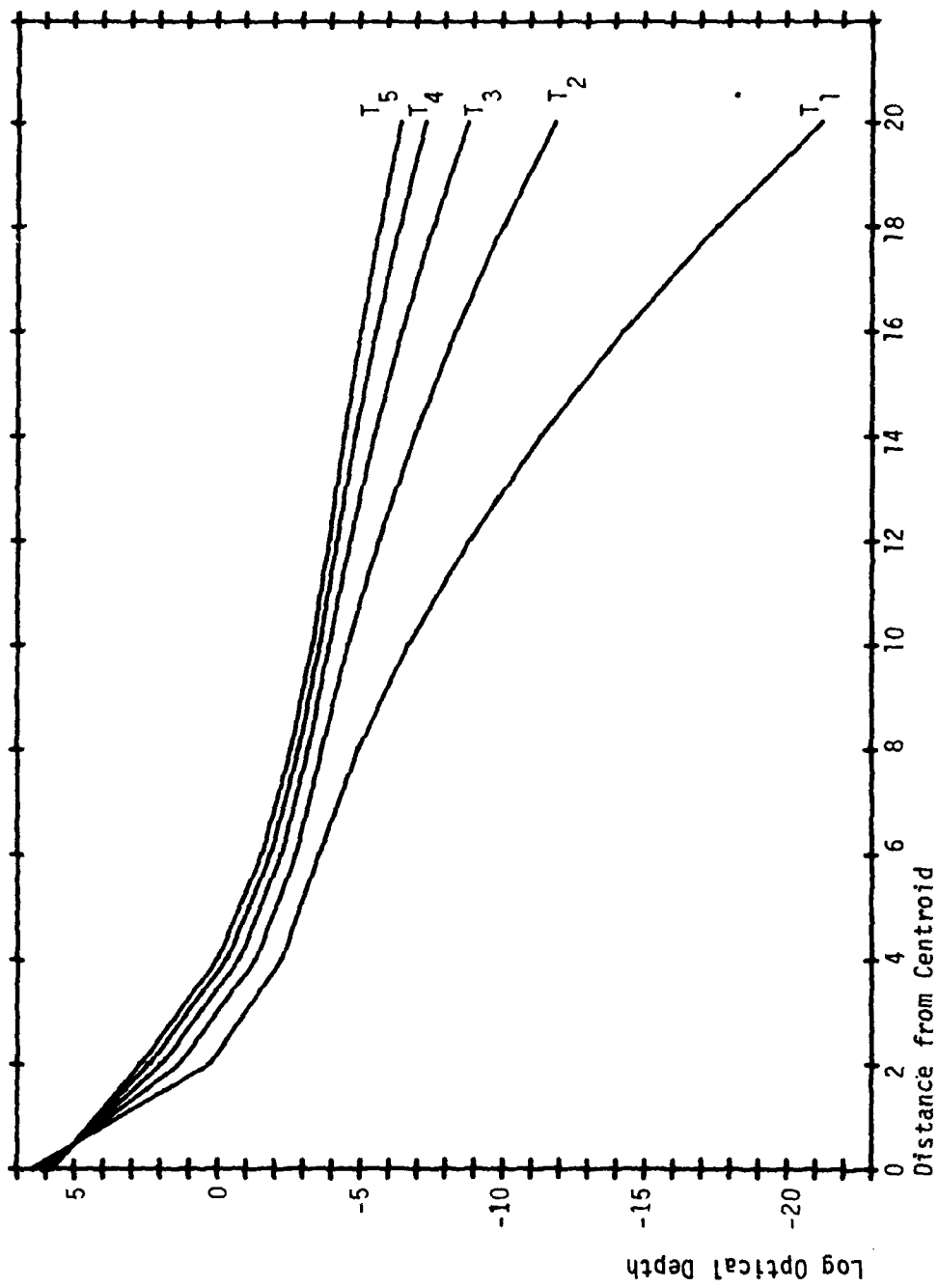


Figure 28. Optical depth versus distance,  $n(r) = 1/r^4$ .

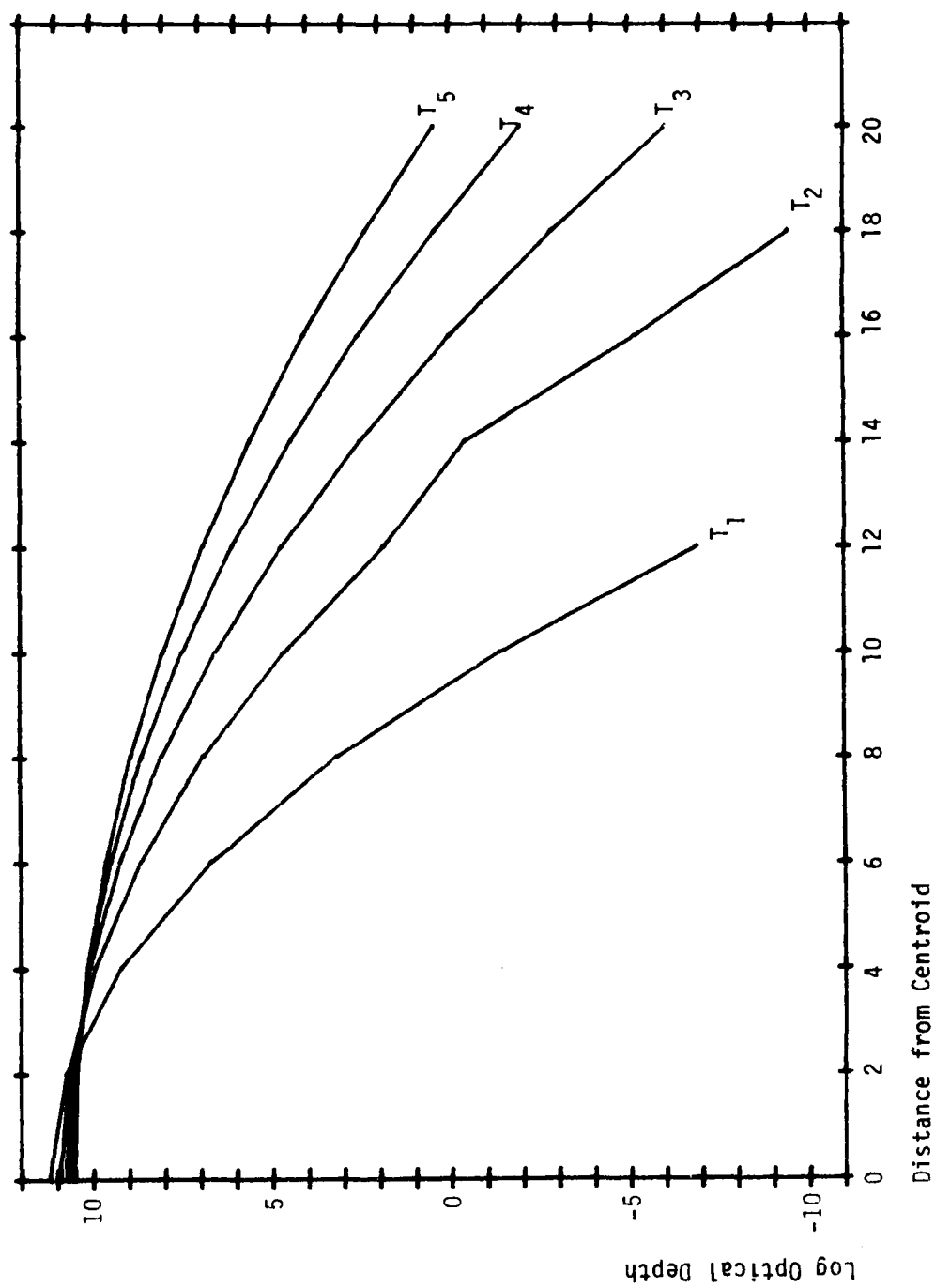


Figure 29. Average optical depth versus distance, first moment average.  
 $n(r) = 1/r^3$ .

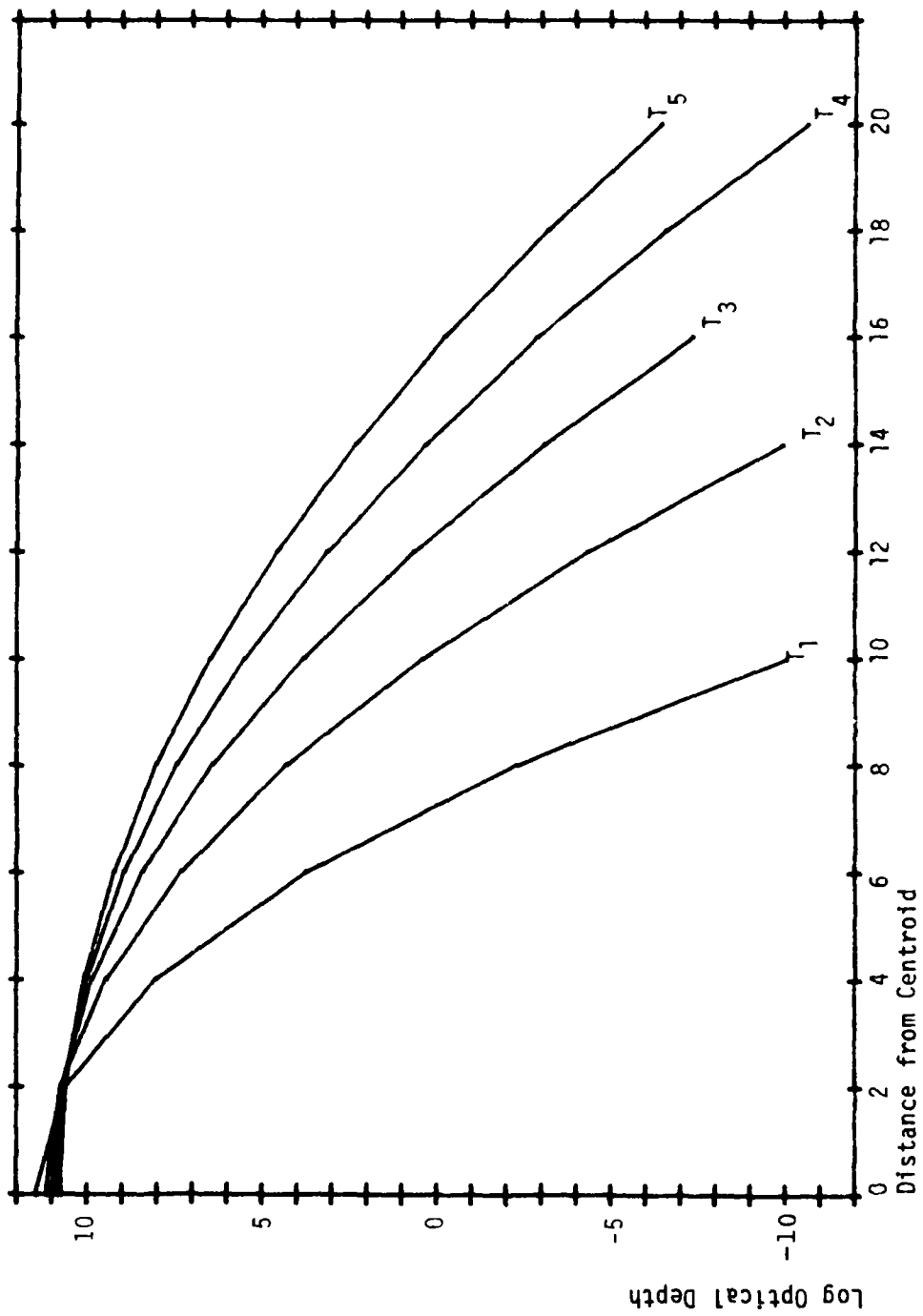


Figure 30. Average optical depth versus distance, second moment average.  
 $n(r) = 1/r^2$ .

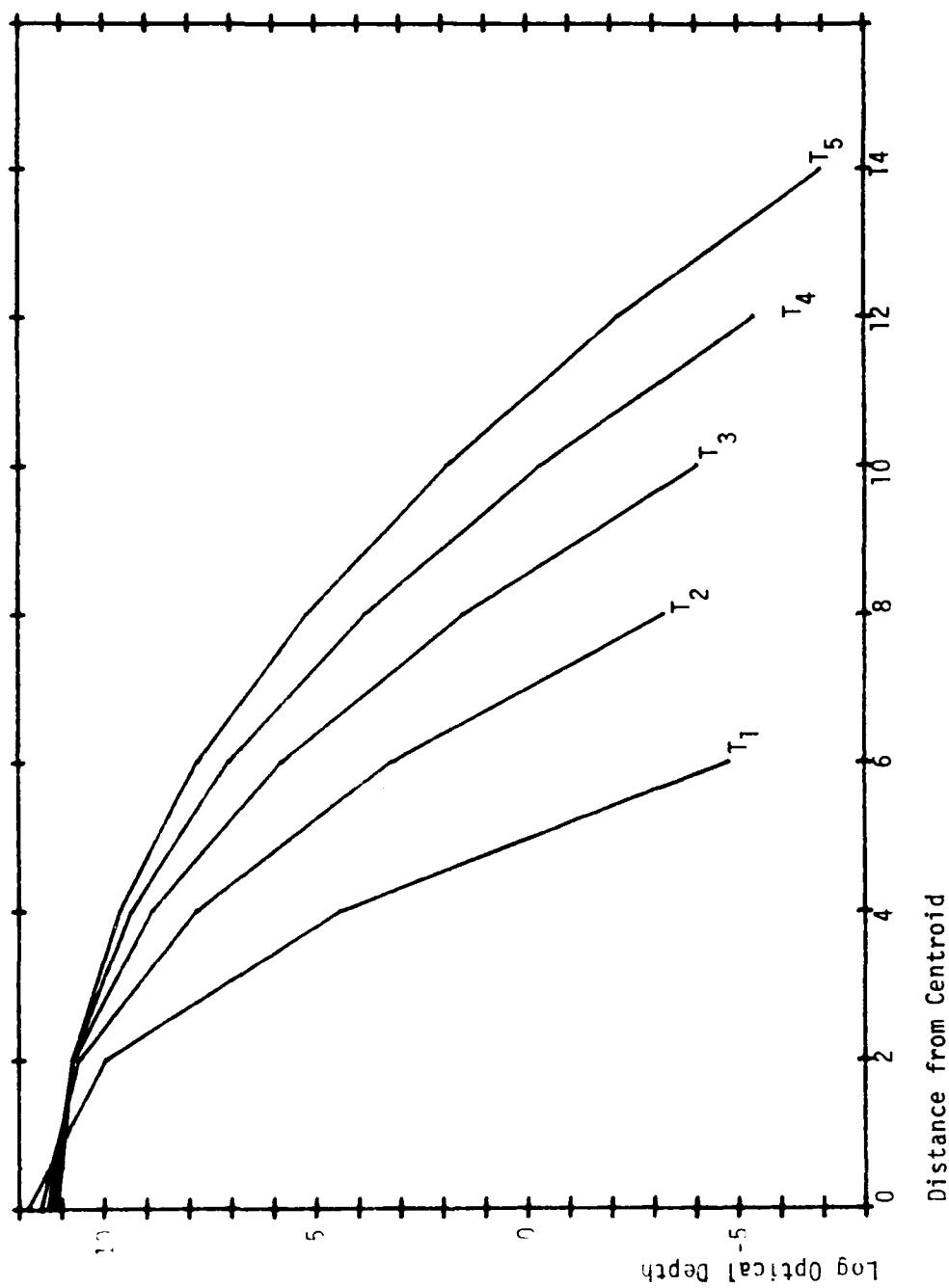


Figure 31. Average optical depth versus distance, third moment average,  
 $n(r) = 1/r^3$ .

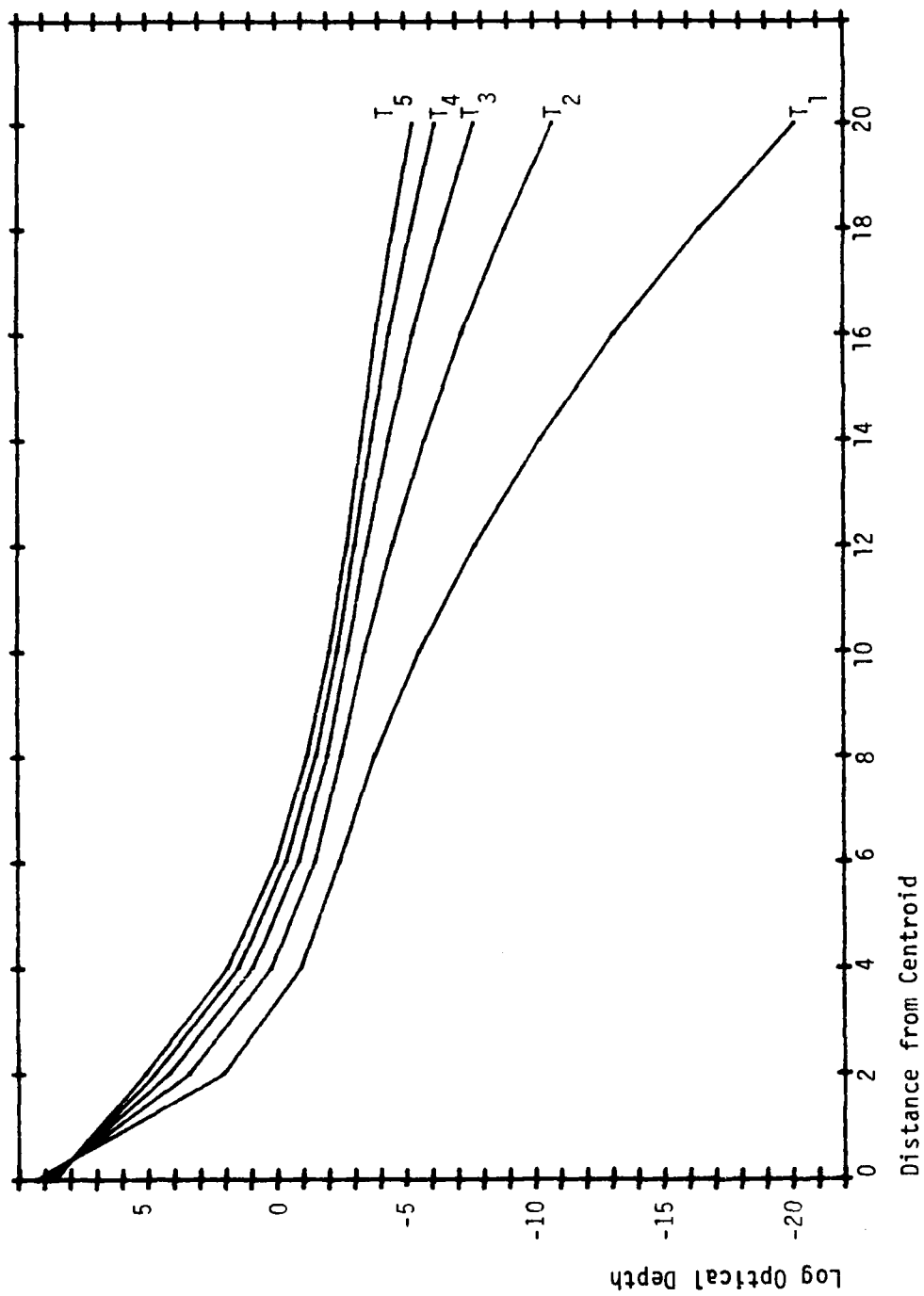


Figure 32. Optical depth versus distance,  $n(r) = 1/r^3$ .

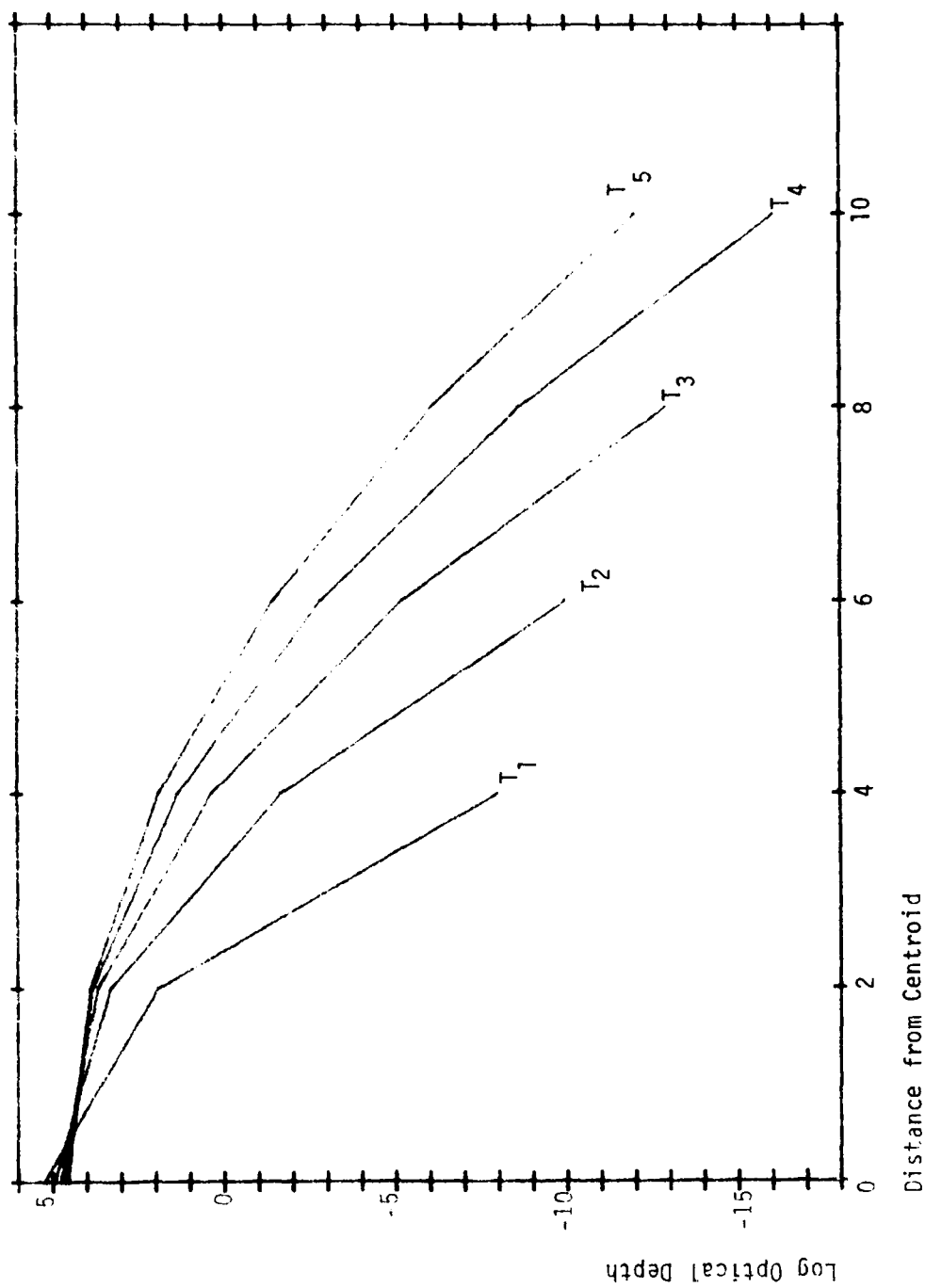


Figure 33. Average optical depth versus distance, second moment average,  $n(r) = \text{Deirmendjian haze } H$ .

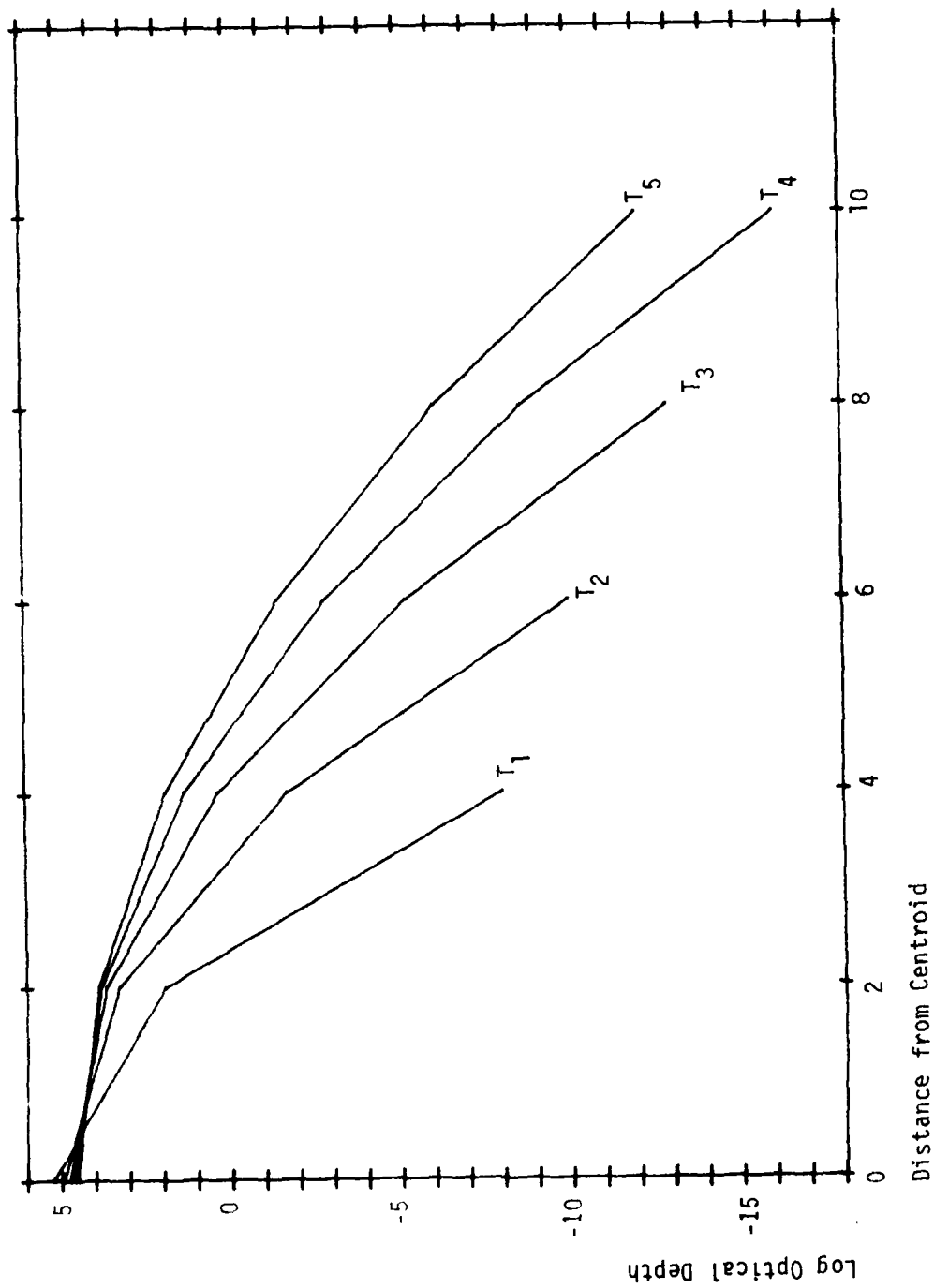


Figure 34. Average optical depth versus distance, second moment average,  
 $n(r)$  = Deirmendjian haze H.

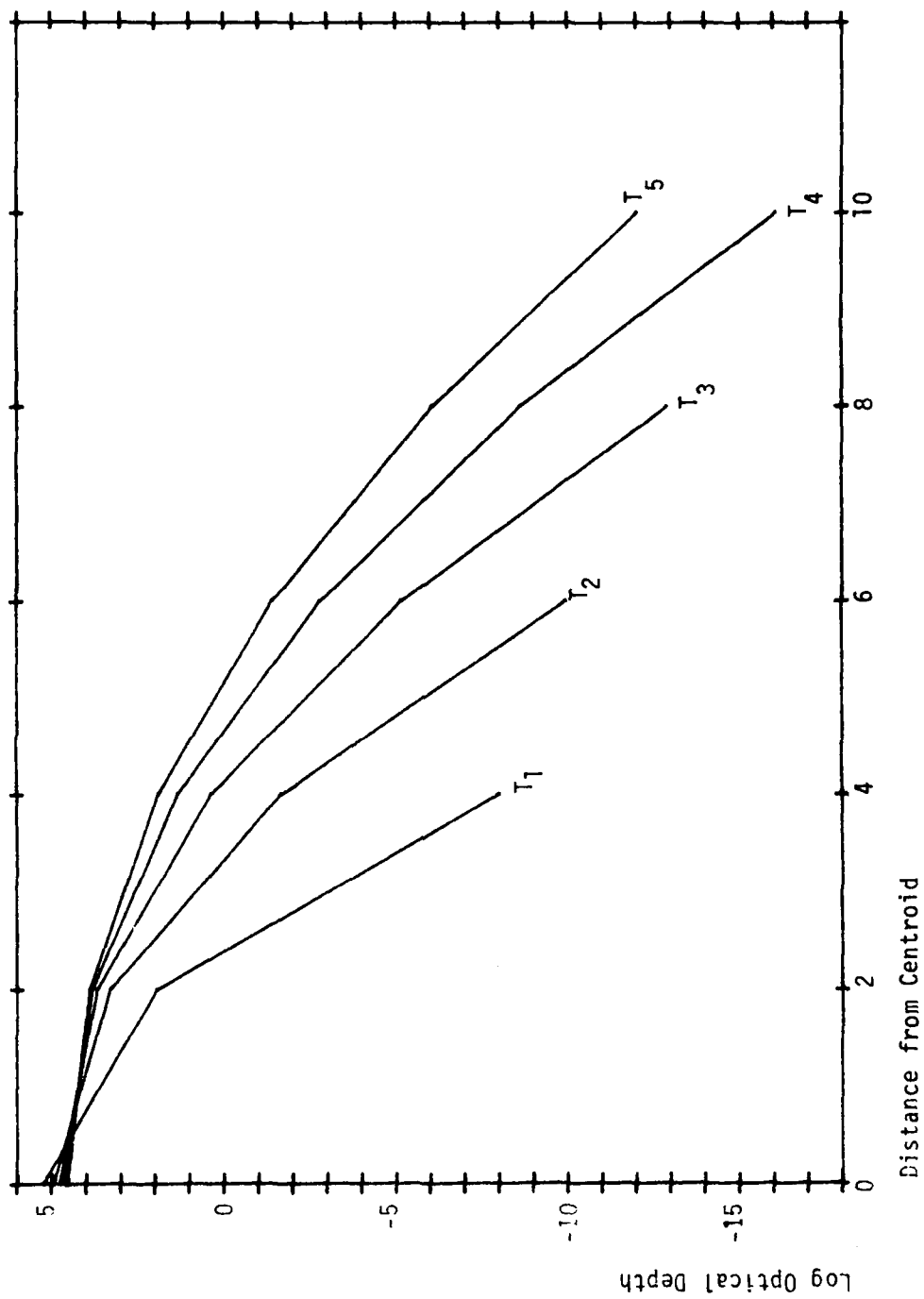


Figure 35. Average optical depth versus distance, third moment average,  $n(r)$  = Deirmendjian haze H.

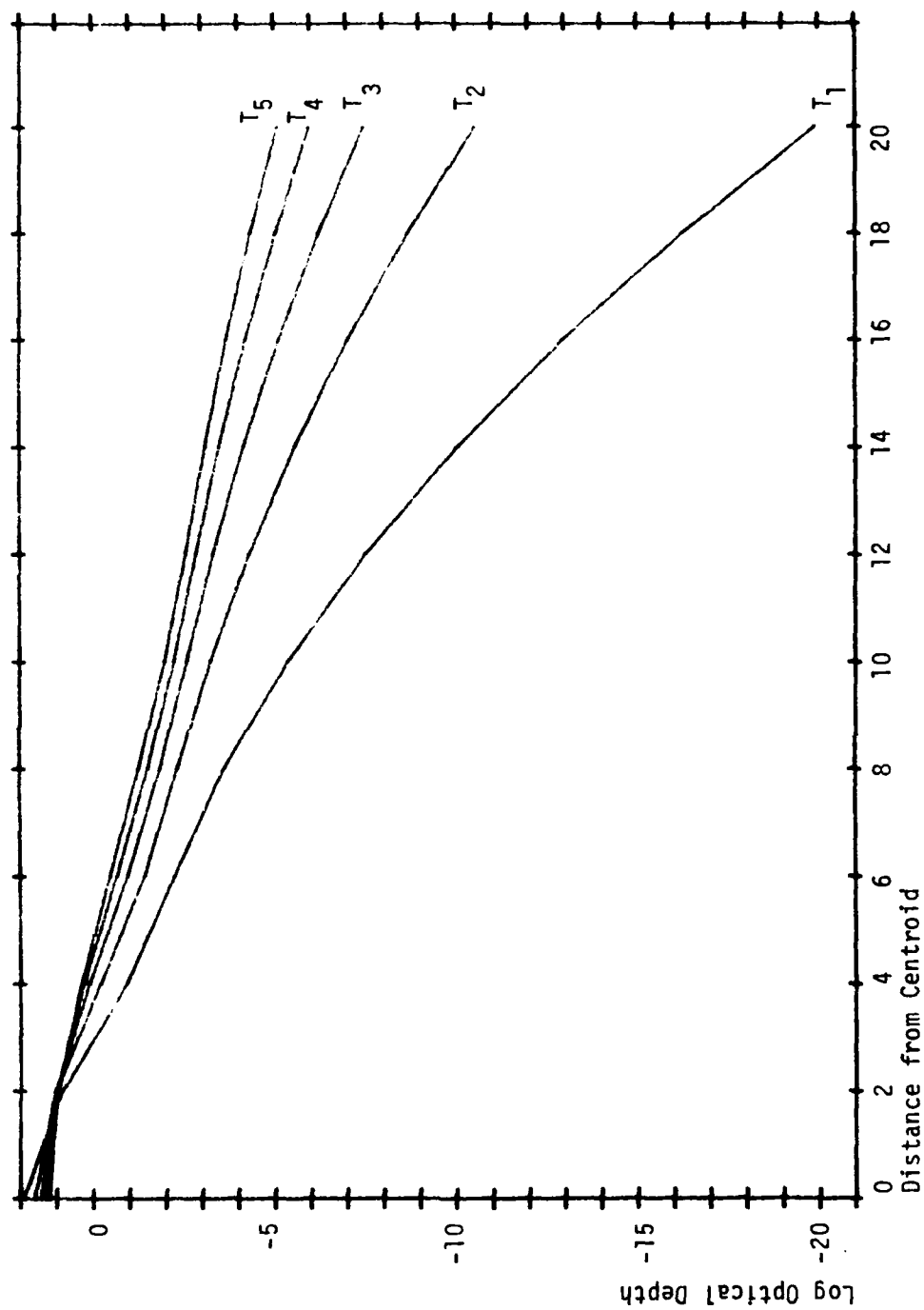


Figure 36. Optical depth versus distance,  $n(r)$  = Deirmendjian haze H.

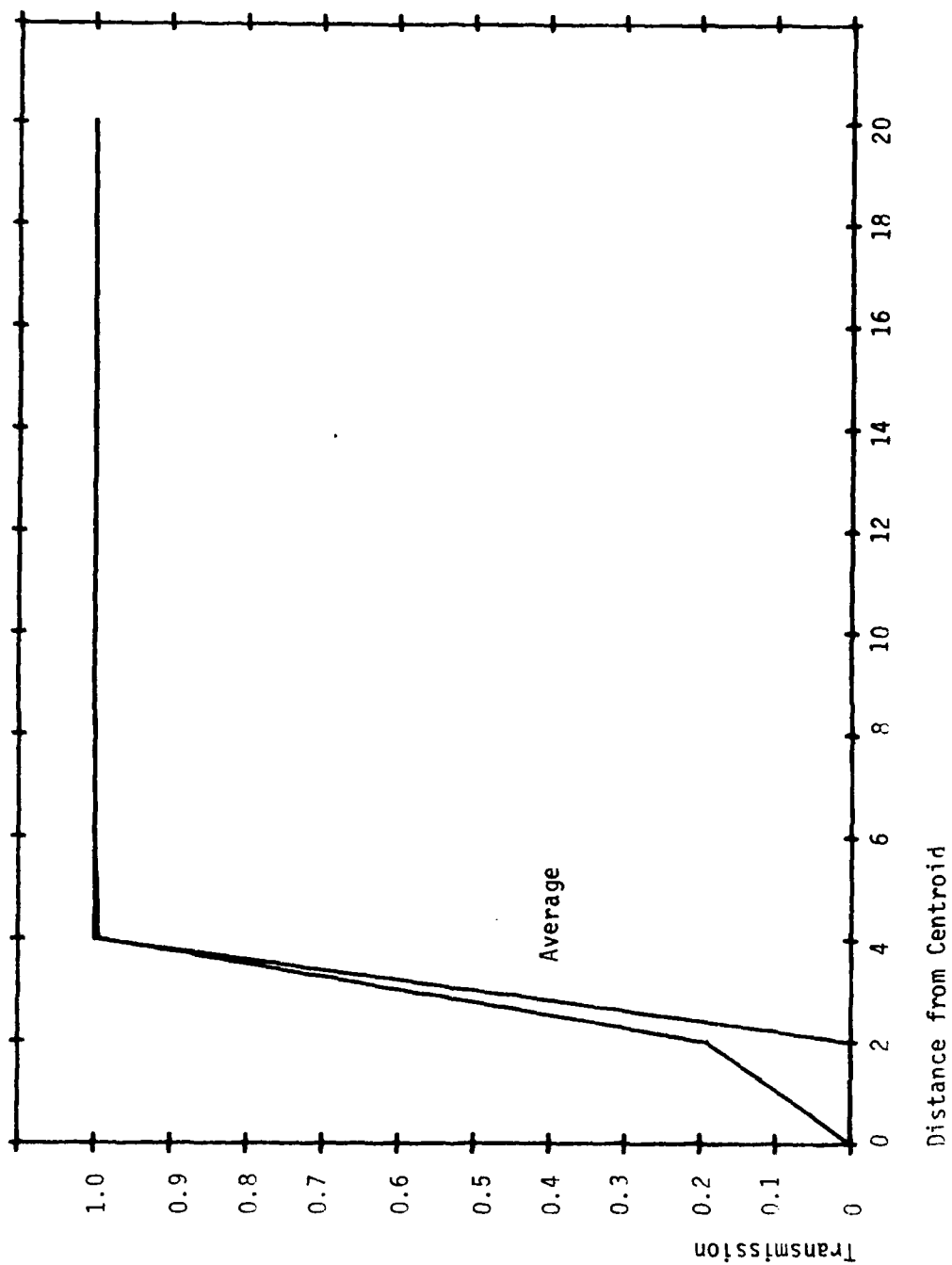


Figure 37. Transmission versus distance, first moment average, time  $T_1$ ,  $n(r) = 1/r^4$ .

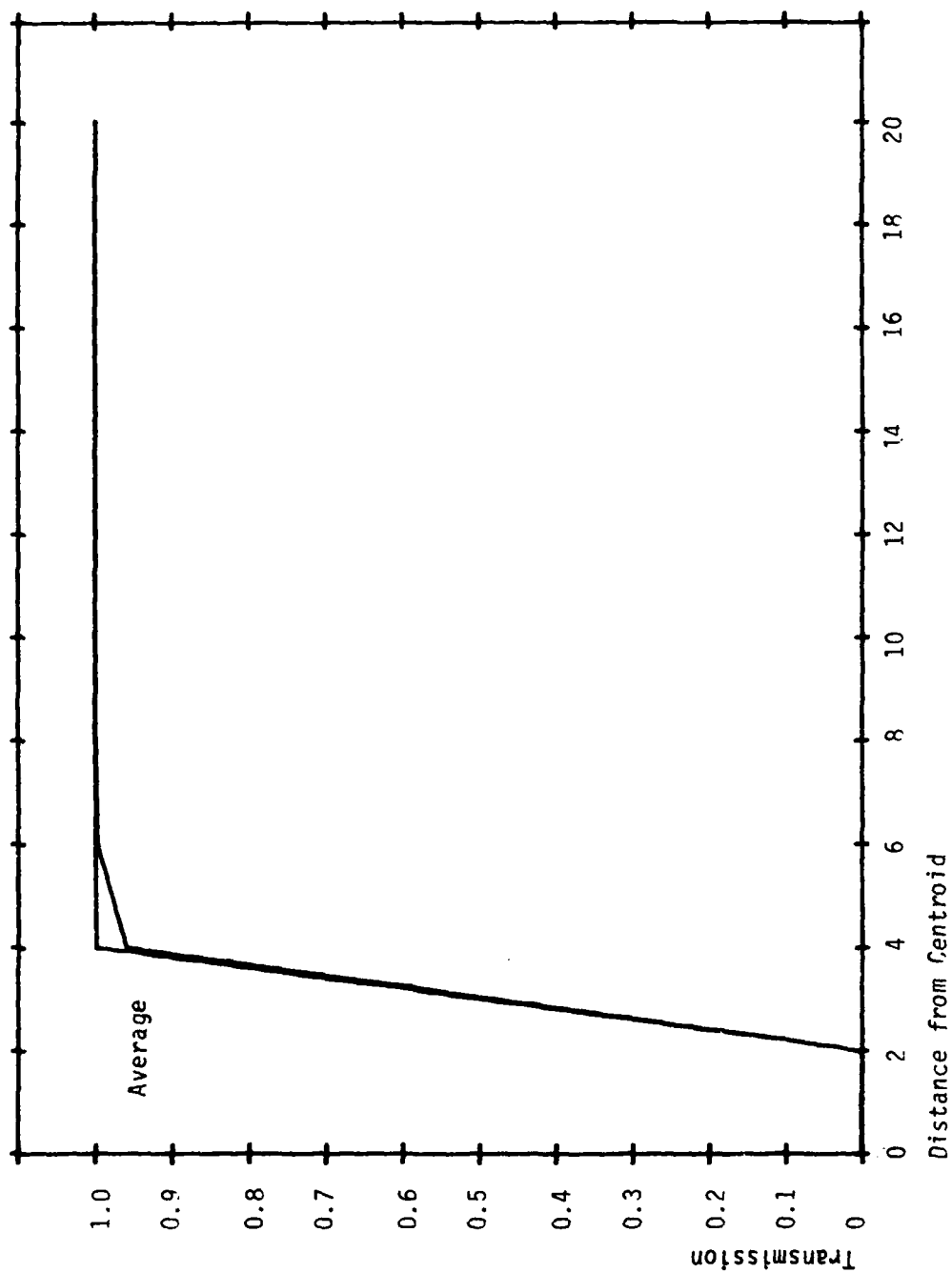


Figure 38. Transmission versus distance, first moment average, time  $T_2$ ,  $n(r) = 1/r^4$ .

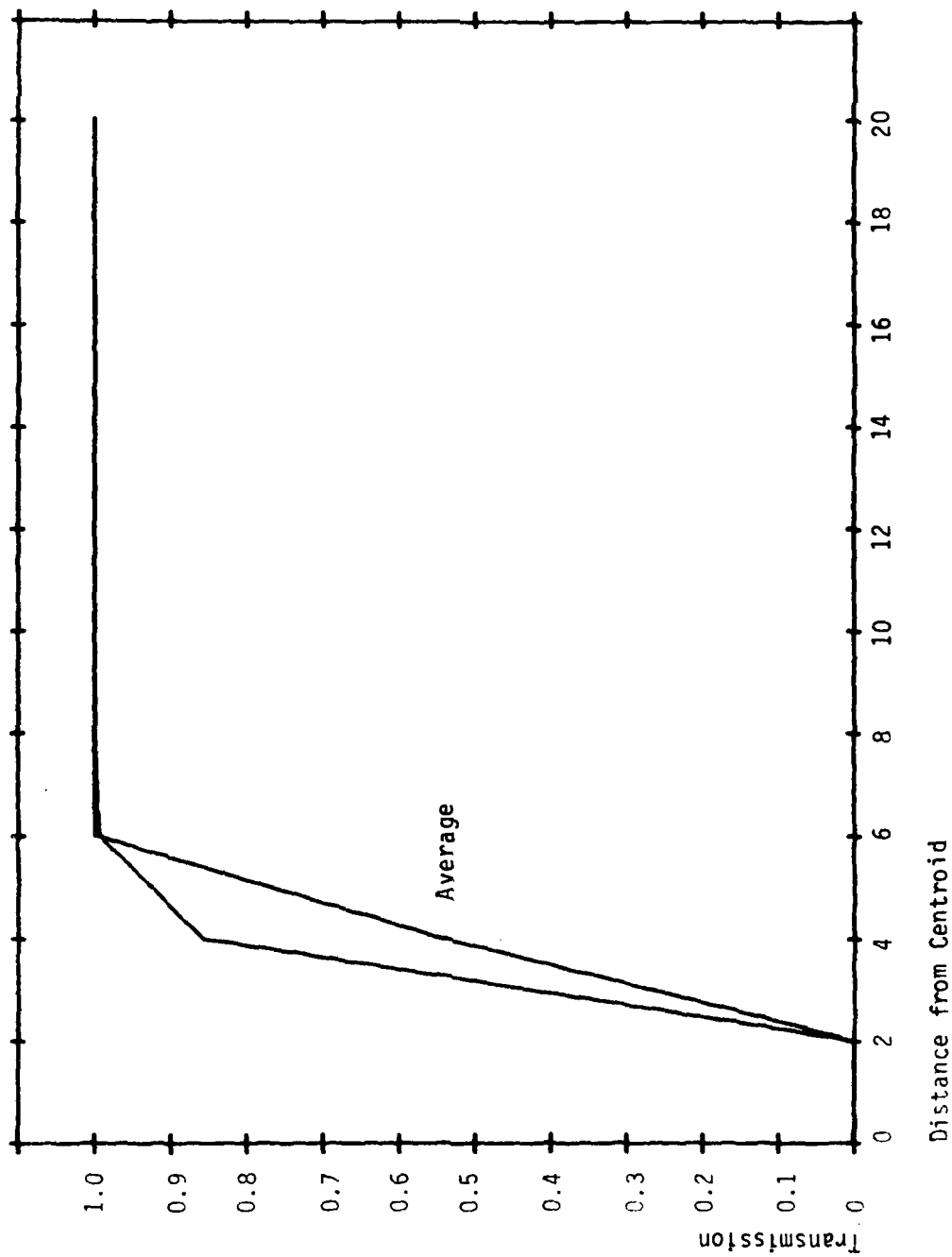
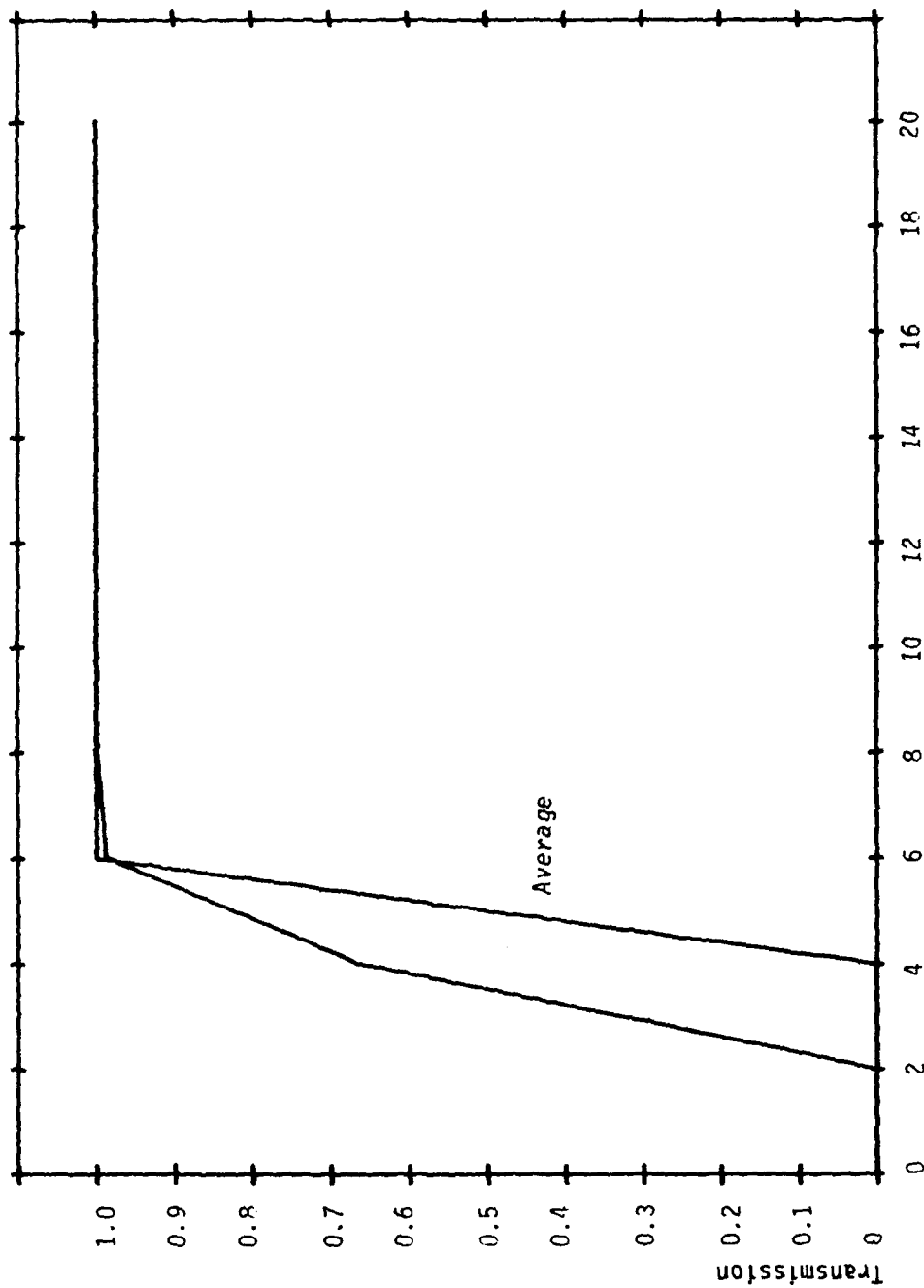


Figure 39. Transmission versus distance, first moment average, time  $T_3$ .  
 $n(r) = 1/r^4$ .



Distance from Centroid  
 Figure 40. Transmission versus distance, first moment average, time  $T_4$ ,  
 $n(r) = 1/r^4$ .

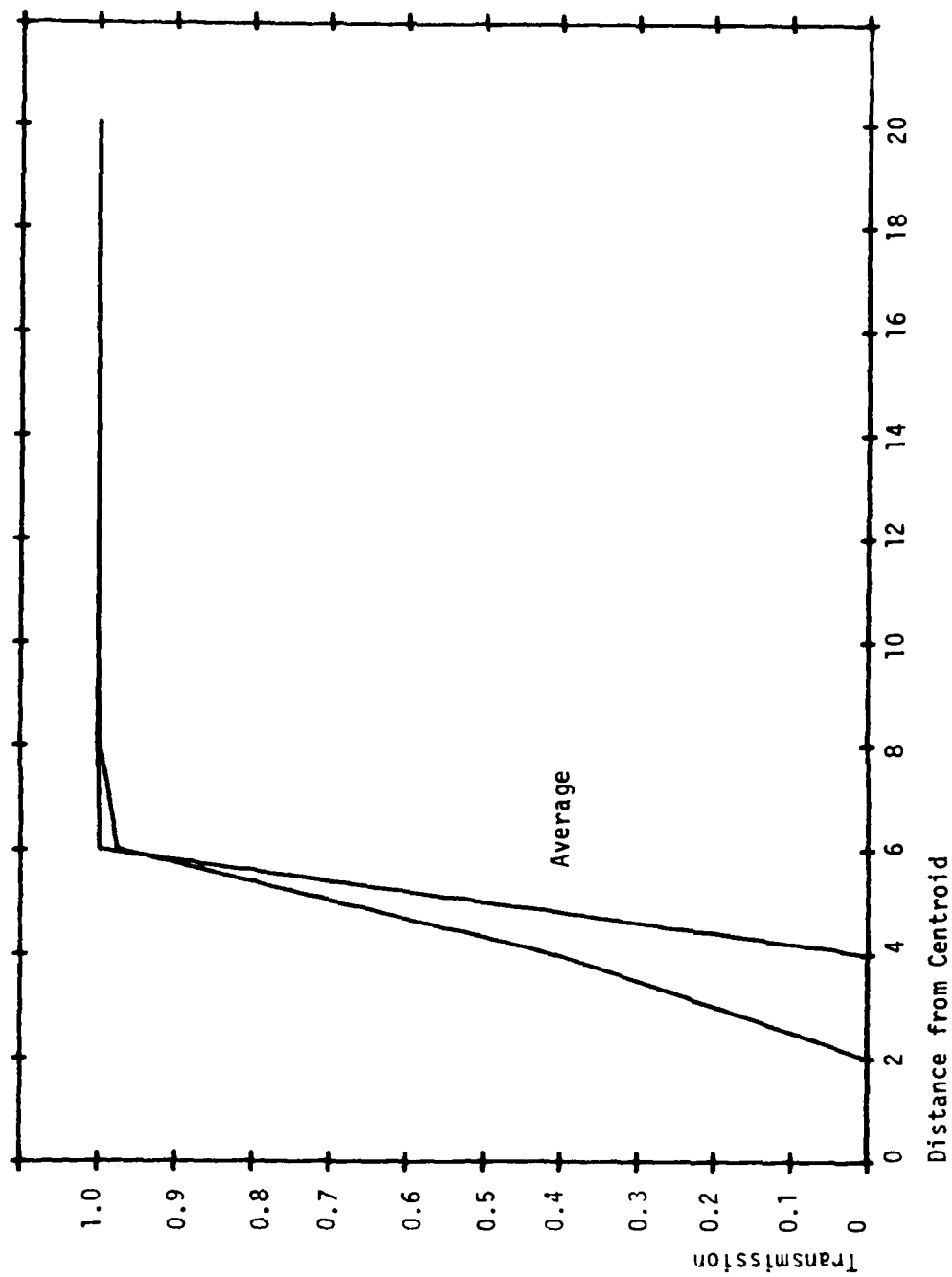


Figure 41. Transmission versus distance, first moment average, time  $T_5$ ,  
 $n(r) = 1/r^4$ .

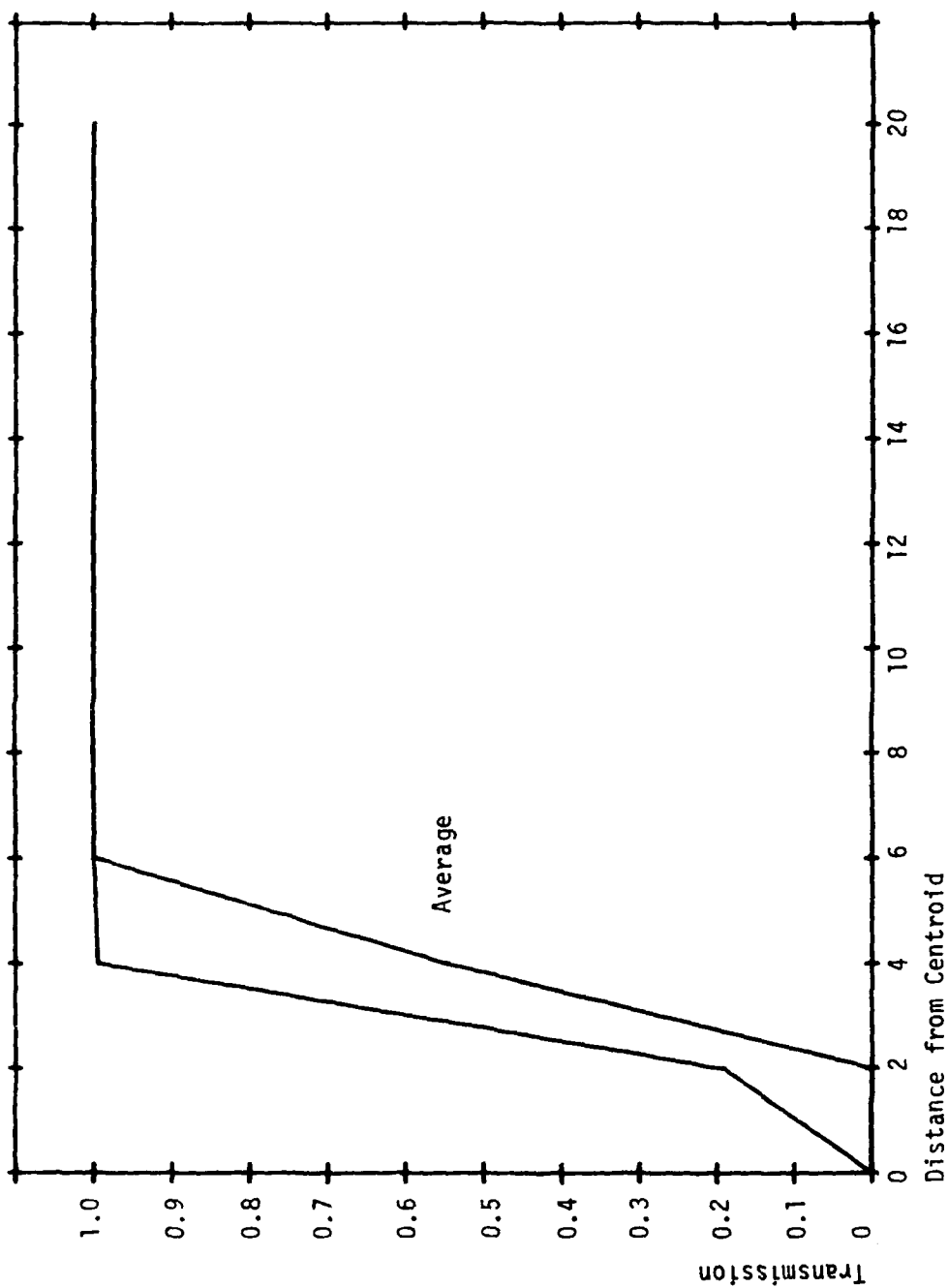


Figure 42. Transmission versus distance, second moment average, time  $T_1$ ,  $n(r) = 1/r^4$ .

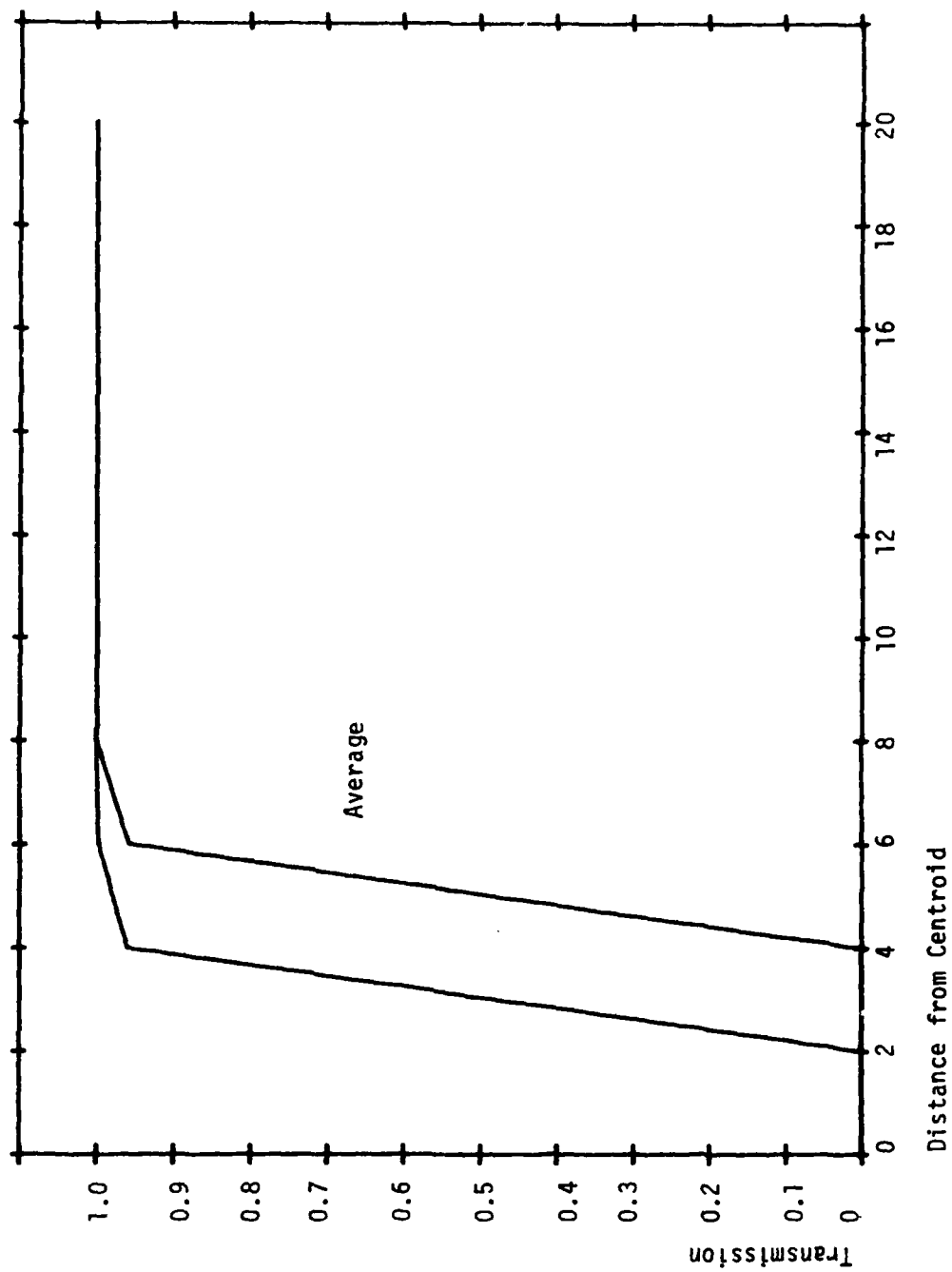


Figure 43. Transmission versus distance, second moment average, time  $T_2$ ,  $n(r) = 1/r^4$ .

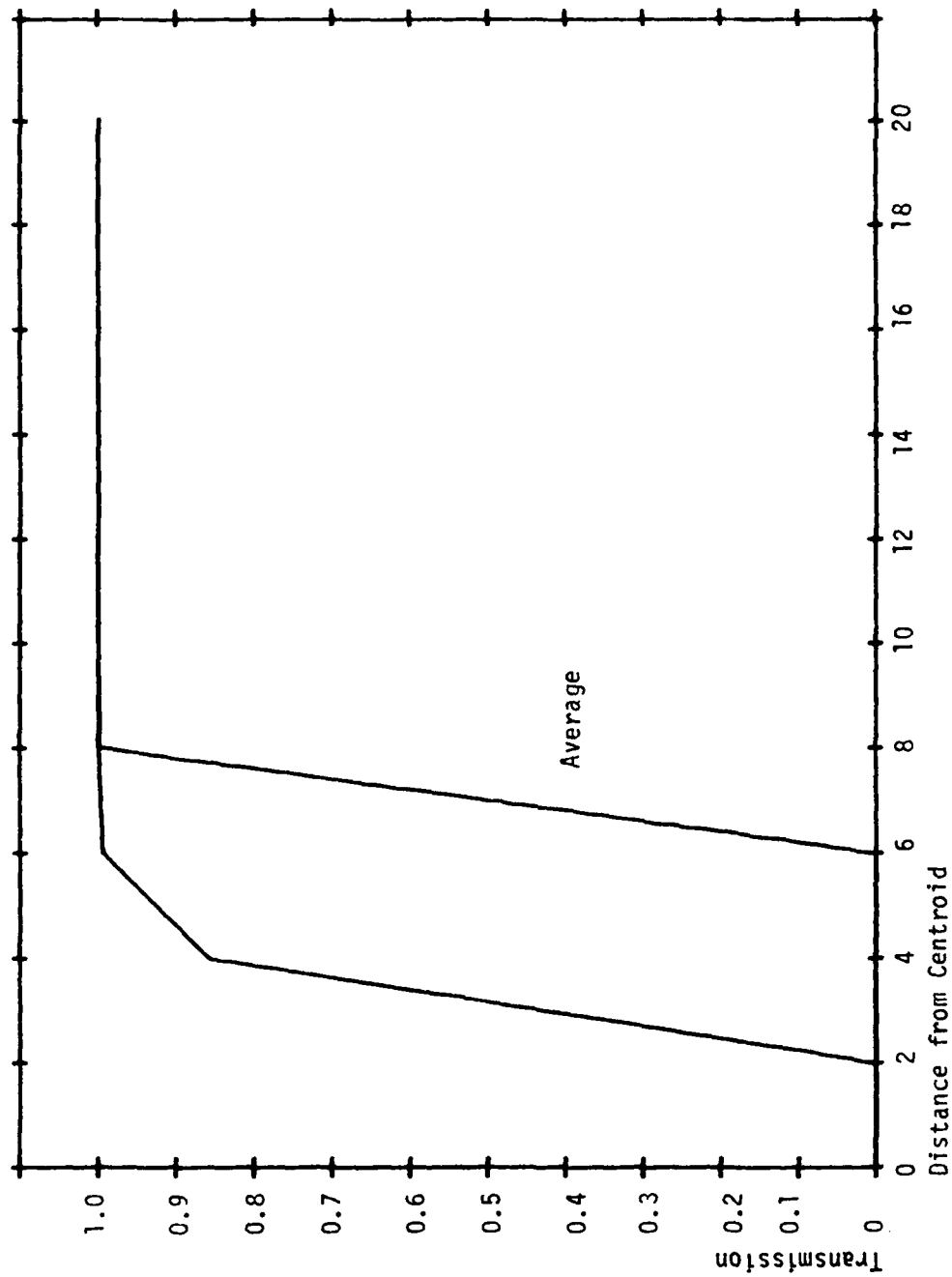


Figure 44. Transmission versus distance, second moment average, time  $T_3$ ,  
 $n(r) = 1/r^4$ .

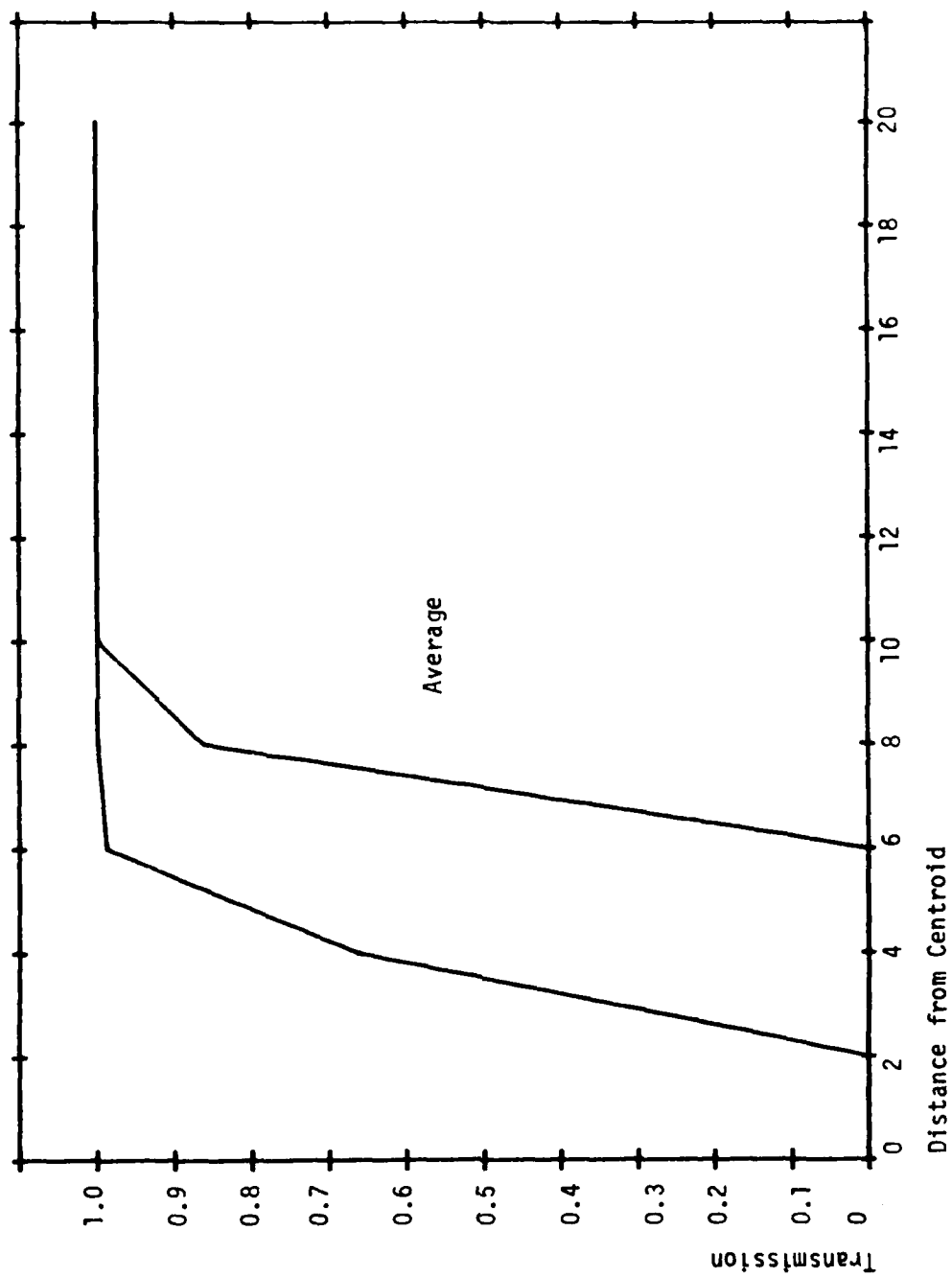


Figure 45. Transmission versus distance, second moment average, time  $T_4$ .  
 $n(r) = 1/r^4$ .

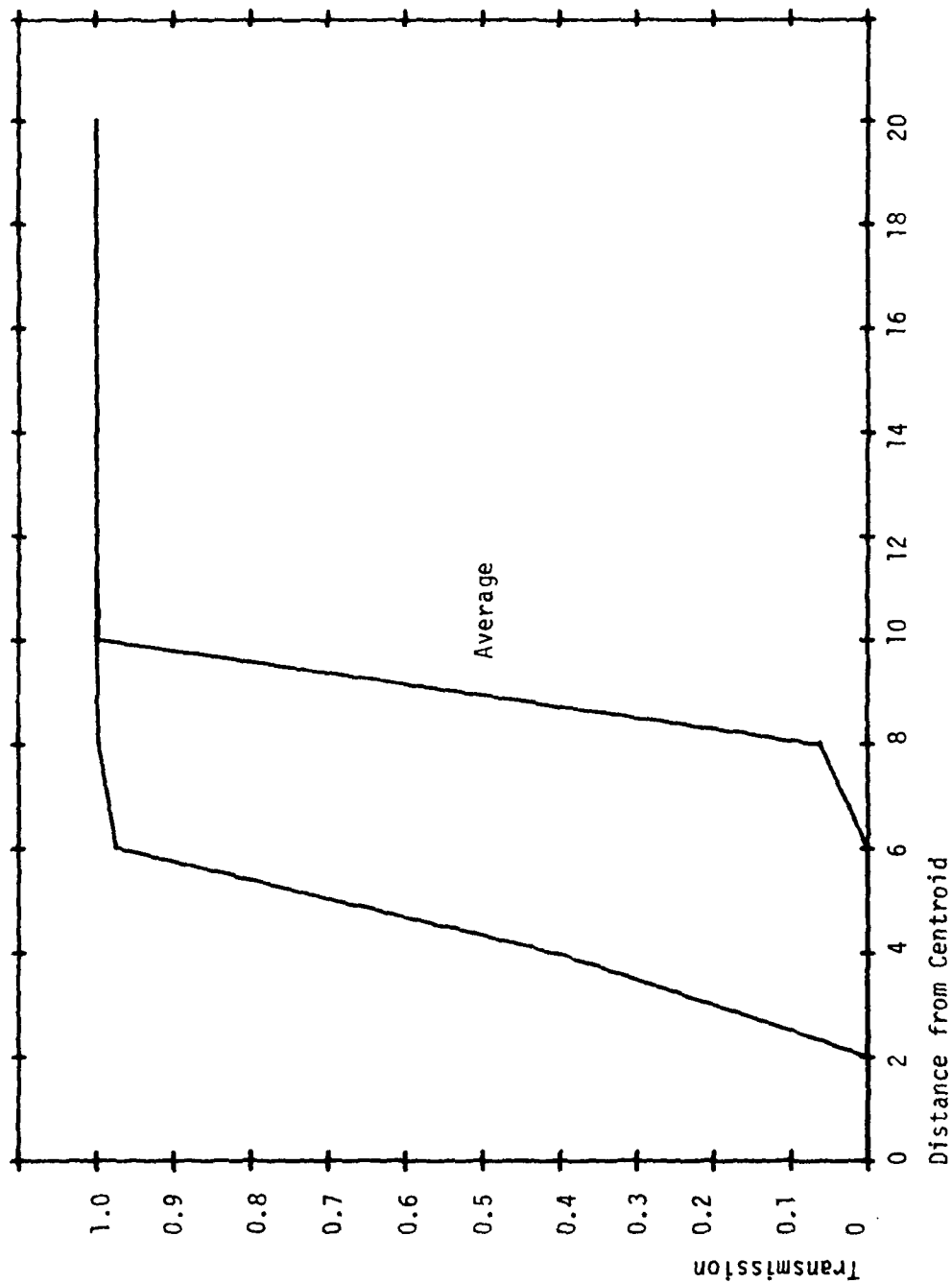


Figure 46. Transmission versus distance, second moment average, time  $T_5$ ,  
 $n(r) = 1/r^4$ .

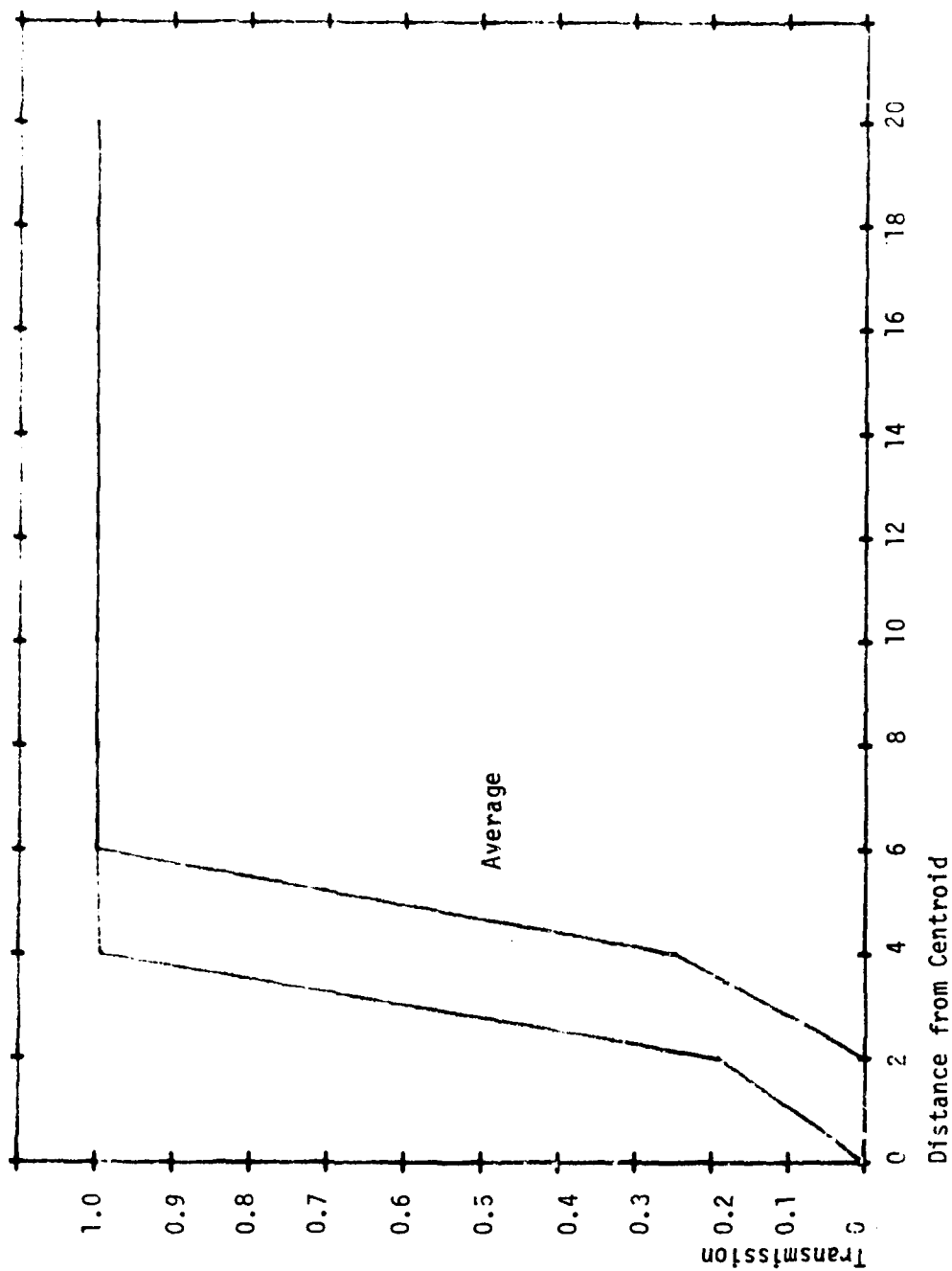


Figure 47. Transmission versus distance, third moment average, time  $T_1$ ,  
 $n(r) = 1/r^4$ .

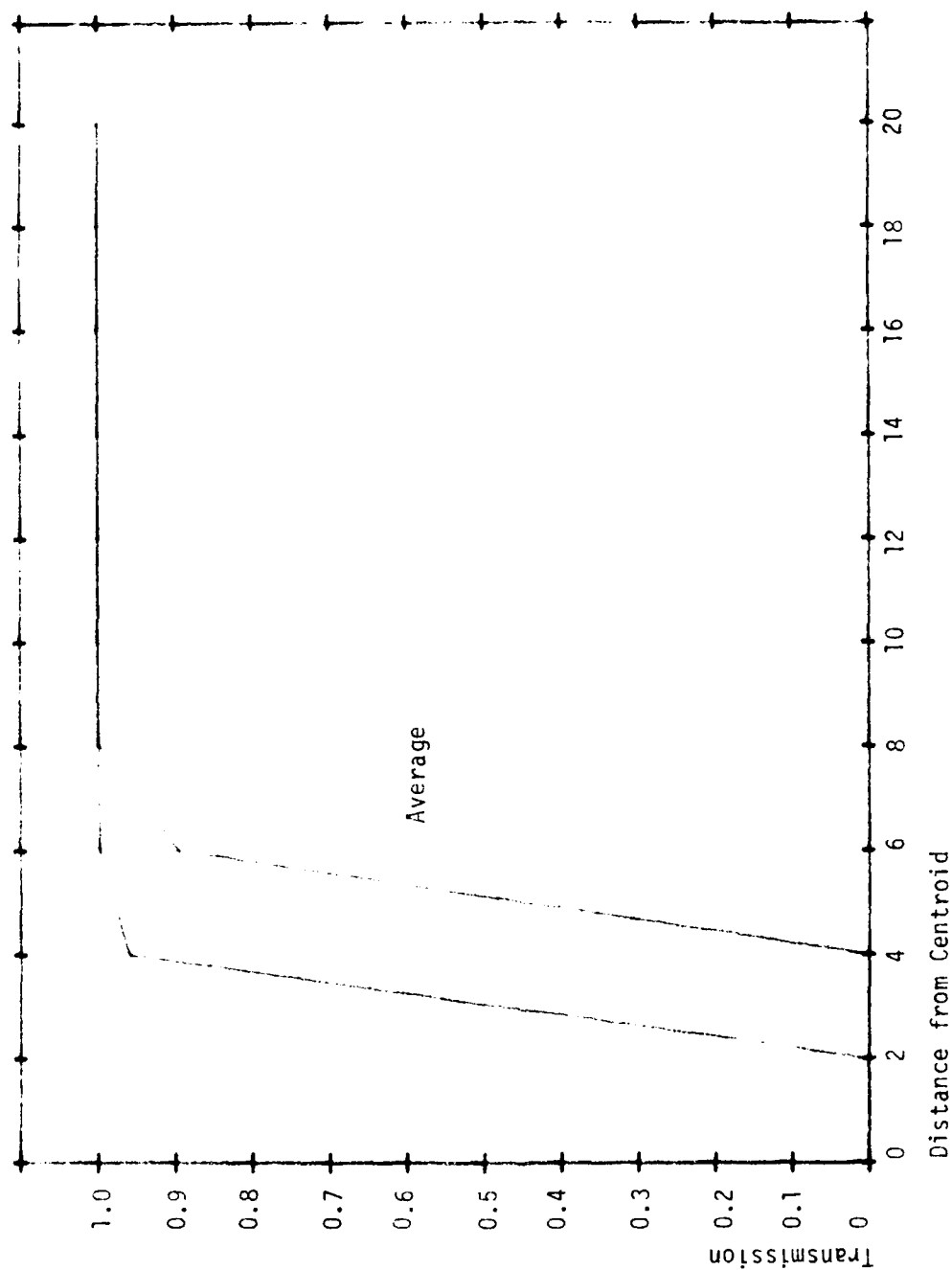


Figure 48. Transmission versus distance, third moment average, time  $T_2$ ,  
 $n(r) = 1/r^4$ .

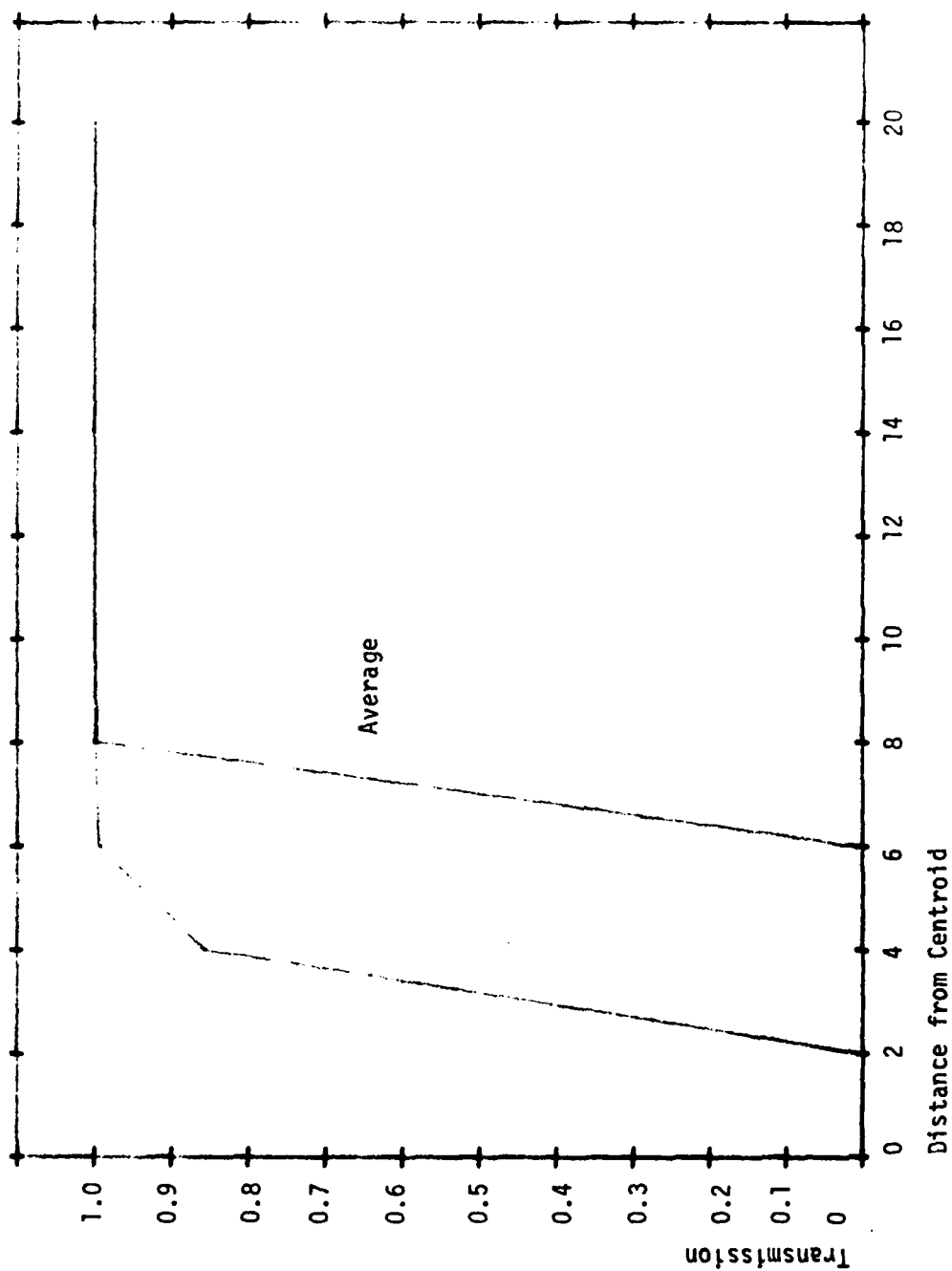


Figure 49. Transmission versus distance, third moment average, time  $T_3$ ,  
 $n(r) = 1/r^4$ .

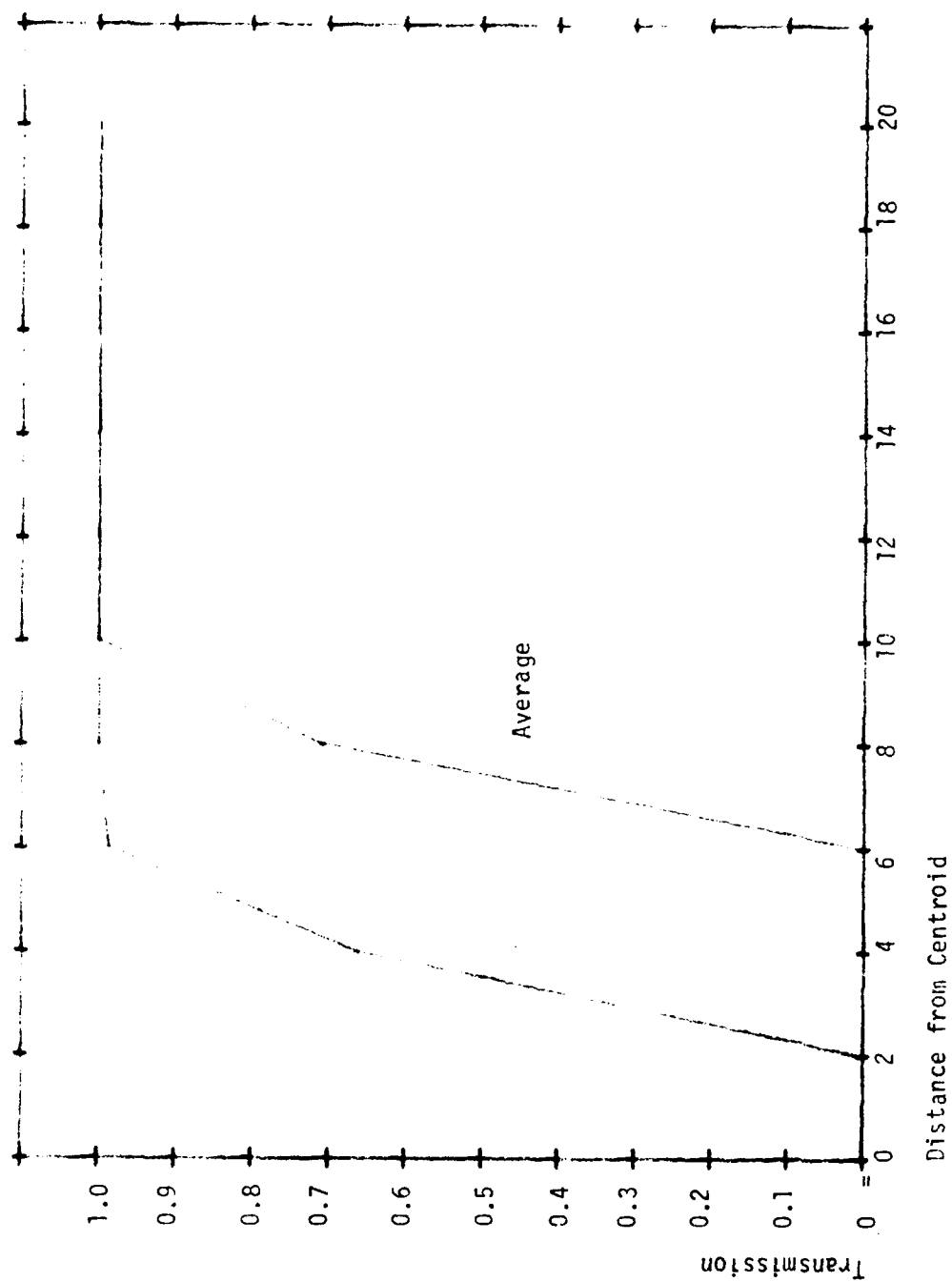


Figure 50. Transmission versus distance, third moment average, time  $T_4$ .

$$n(r) = 1/r^4.$$

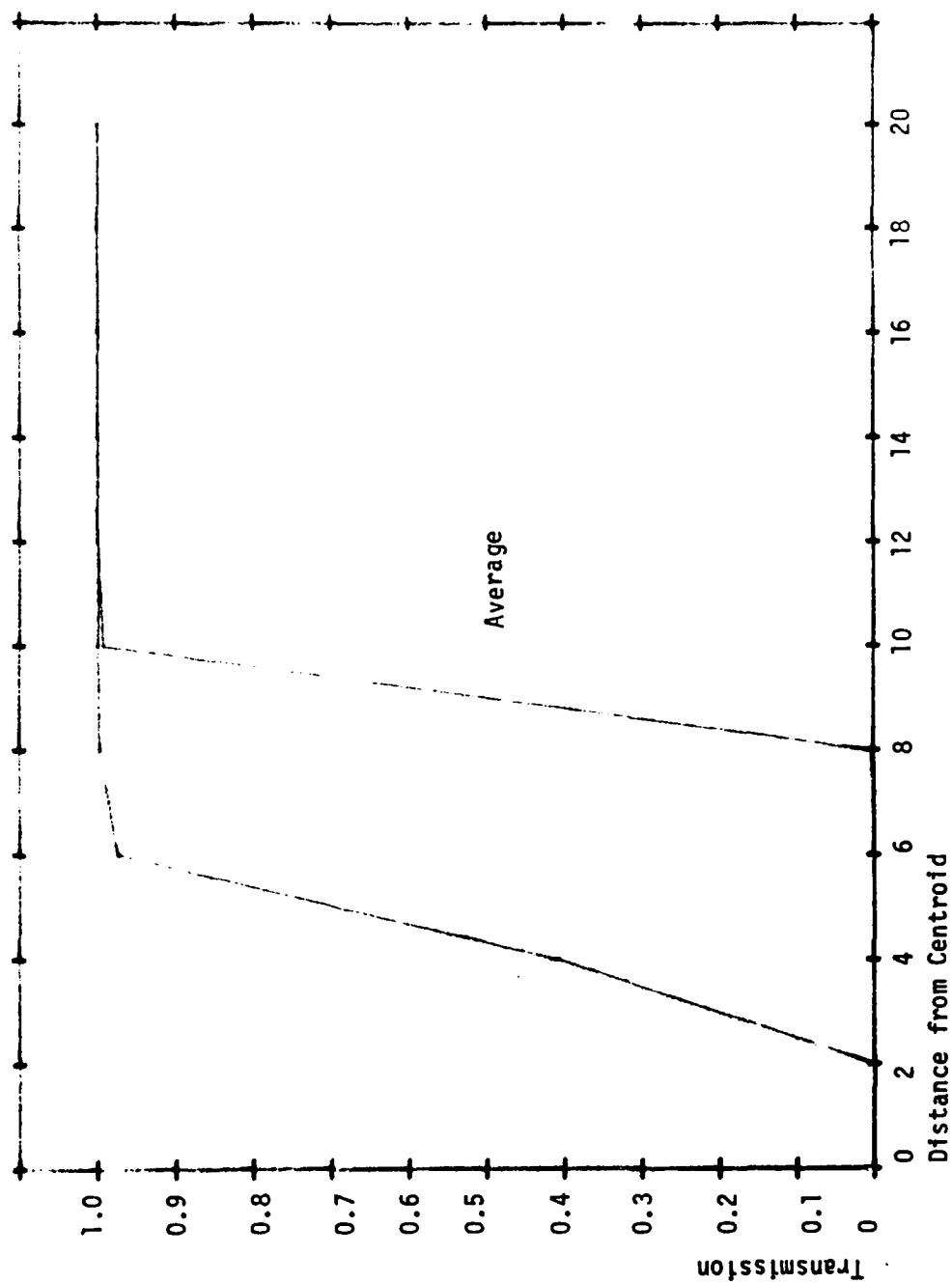


Figure 51. Transmission versus distance, third moment average, time  $T_5$ ,  
 $n(r) = 1/r^4$ .

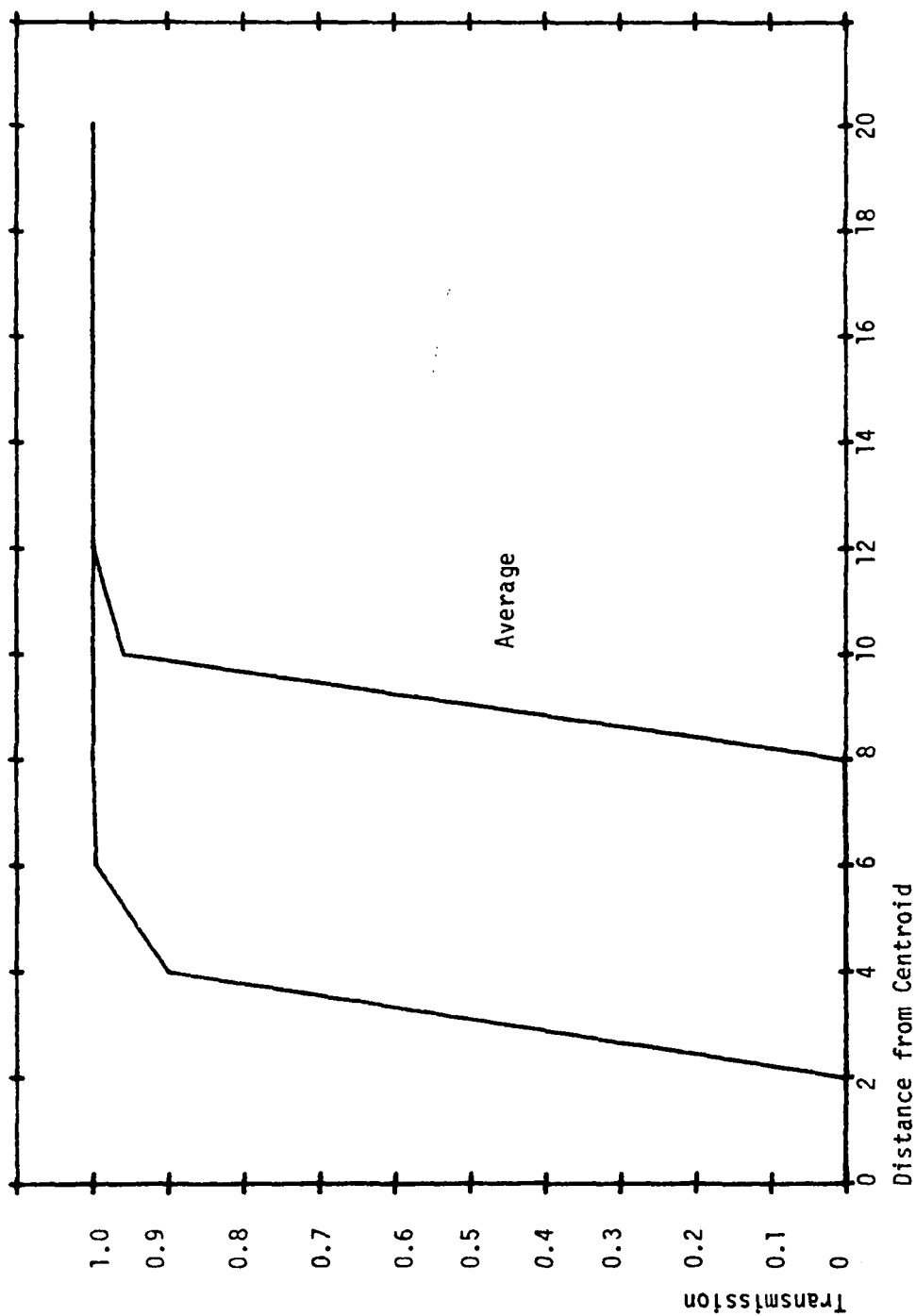


Figure 52. Transmission versus distance, first moment average, time  $T_1$ .

$$n(r) = 1/r^3.$$

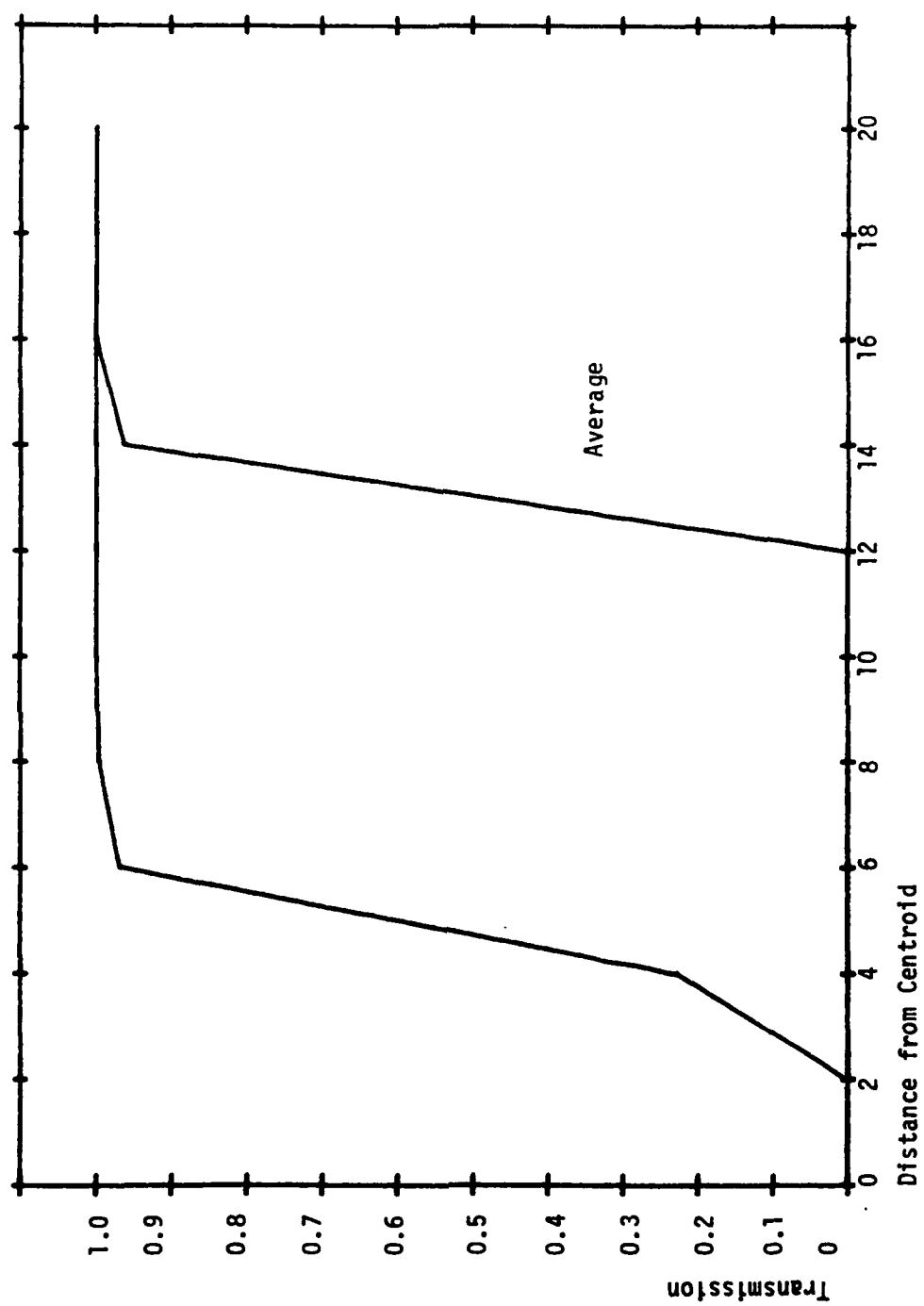


Figure 53. Transmission versus distance, first moment average, time  $T_2$ .

$$n(r) = 1/r^3.$$

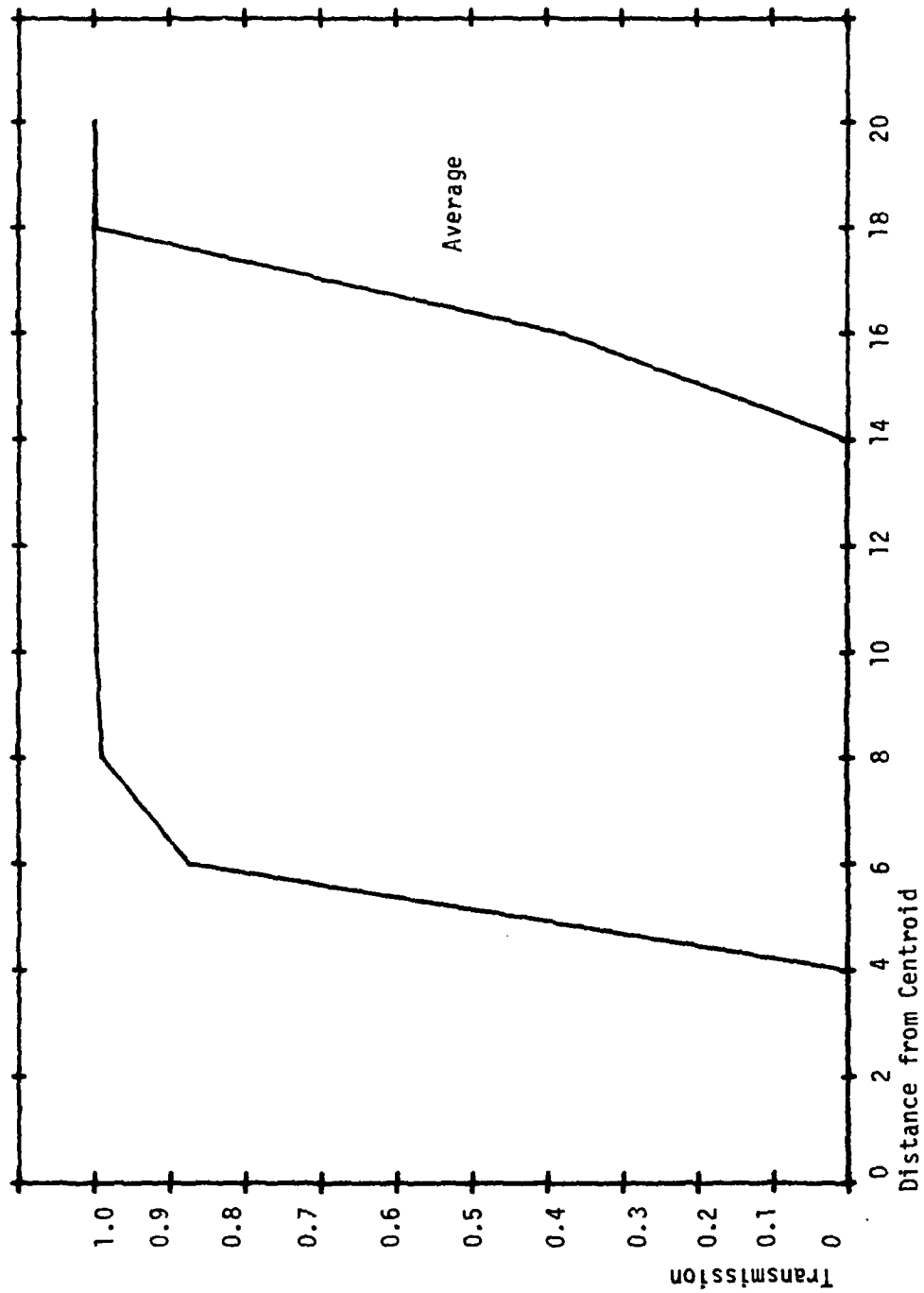


Figure 54. Transmission versus distance, first moment average, time  $T_3$ ,  
 $n(r) = 1/r^3$ .

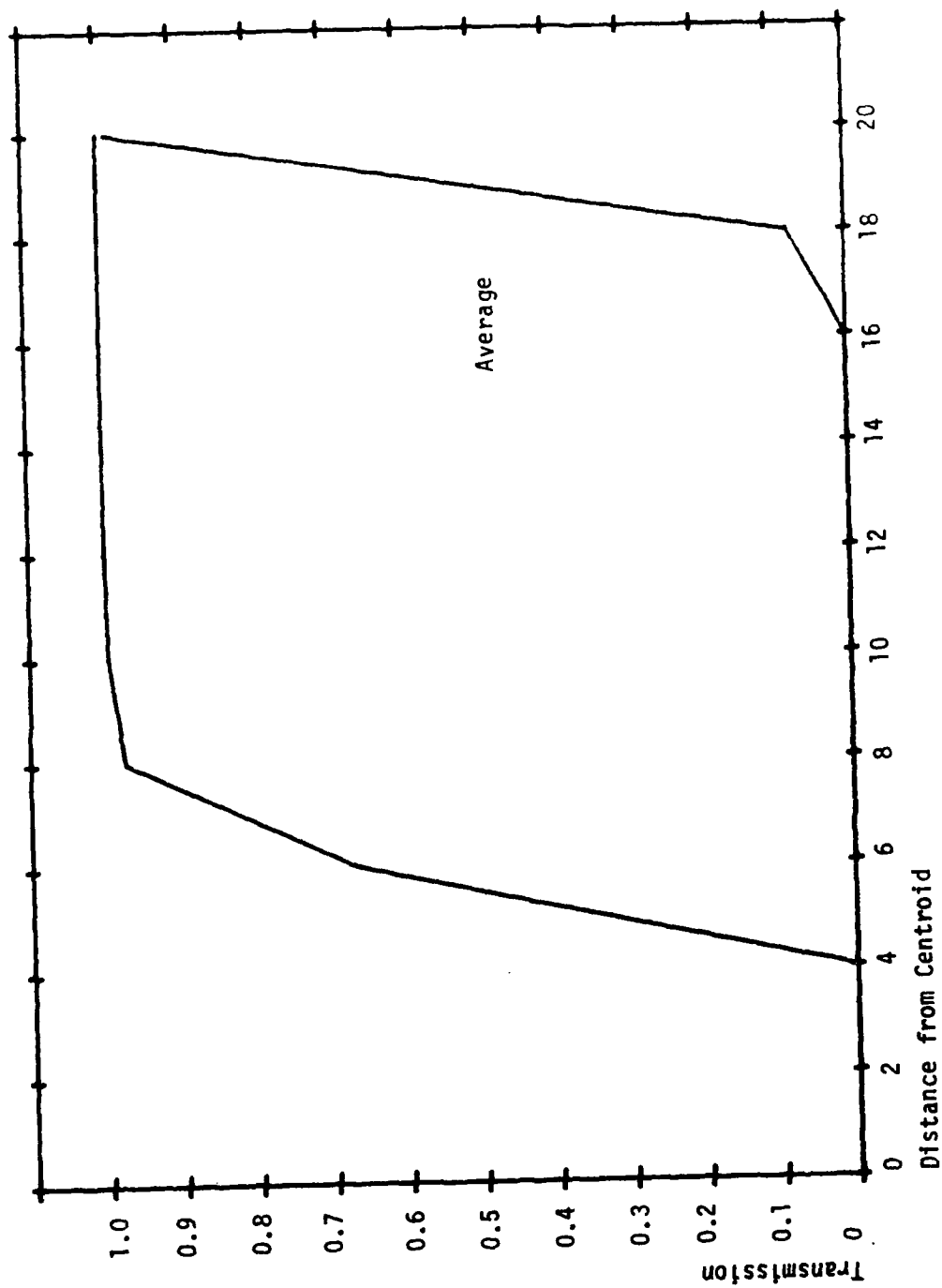


Figure 55. Transmission versus distance, first moment average, time  $T_4$ .  
 $n(r) = 1/r^2$ .

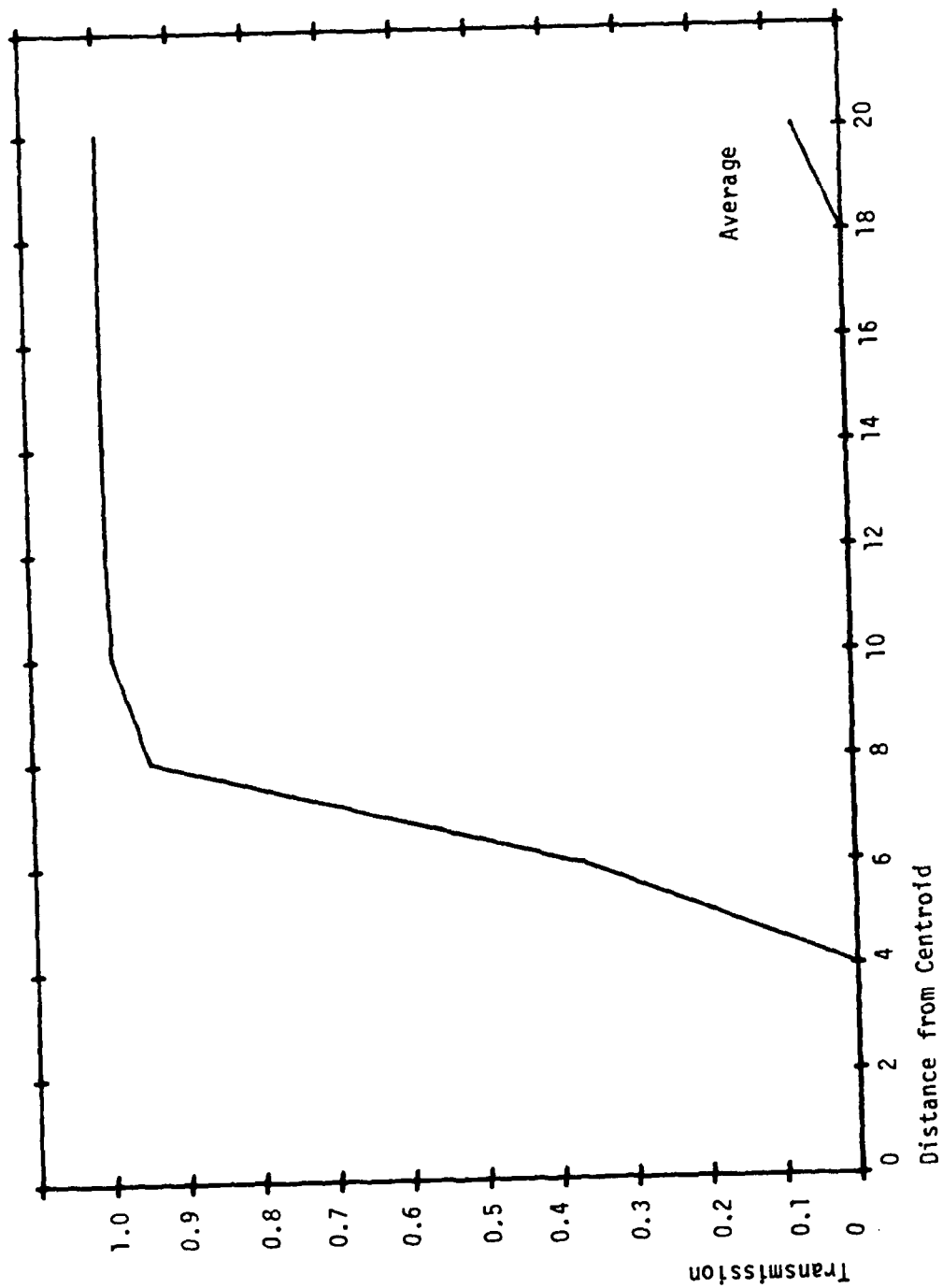


Figure 56. Transmission versus distance, first moment average, time  $T_5$ ,  $n(r) = 1/r^3$ .

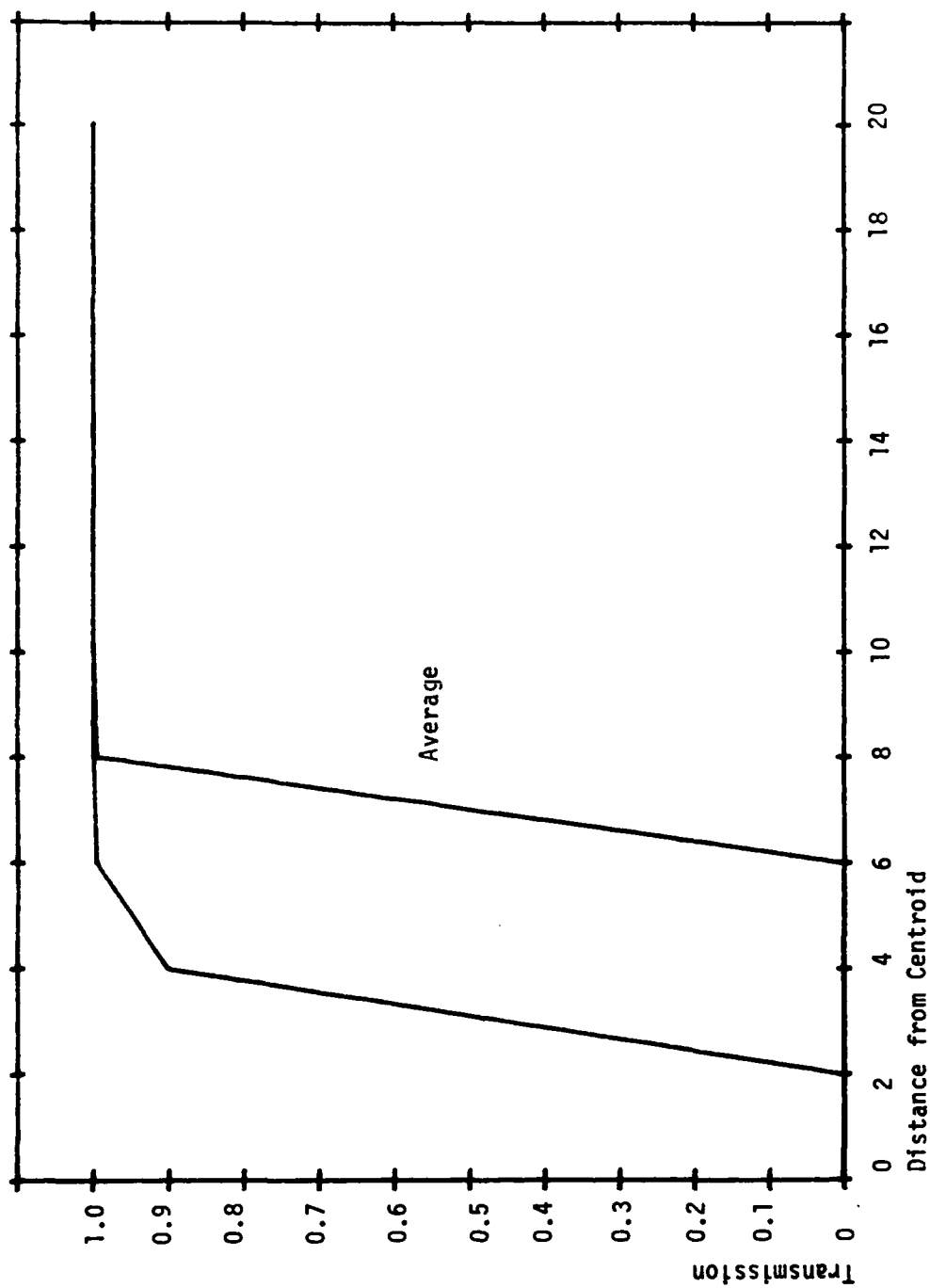


Figure 57. Transmission versus distance, second moment average, time  $T_1$ ,  
 $n(r) = 1/r^3$ .

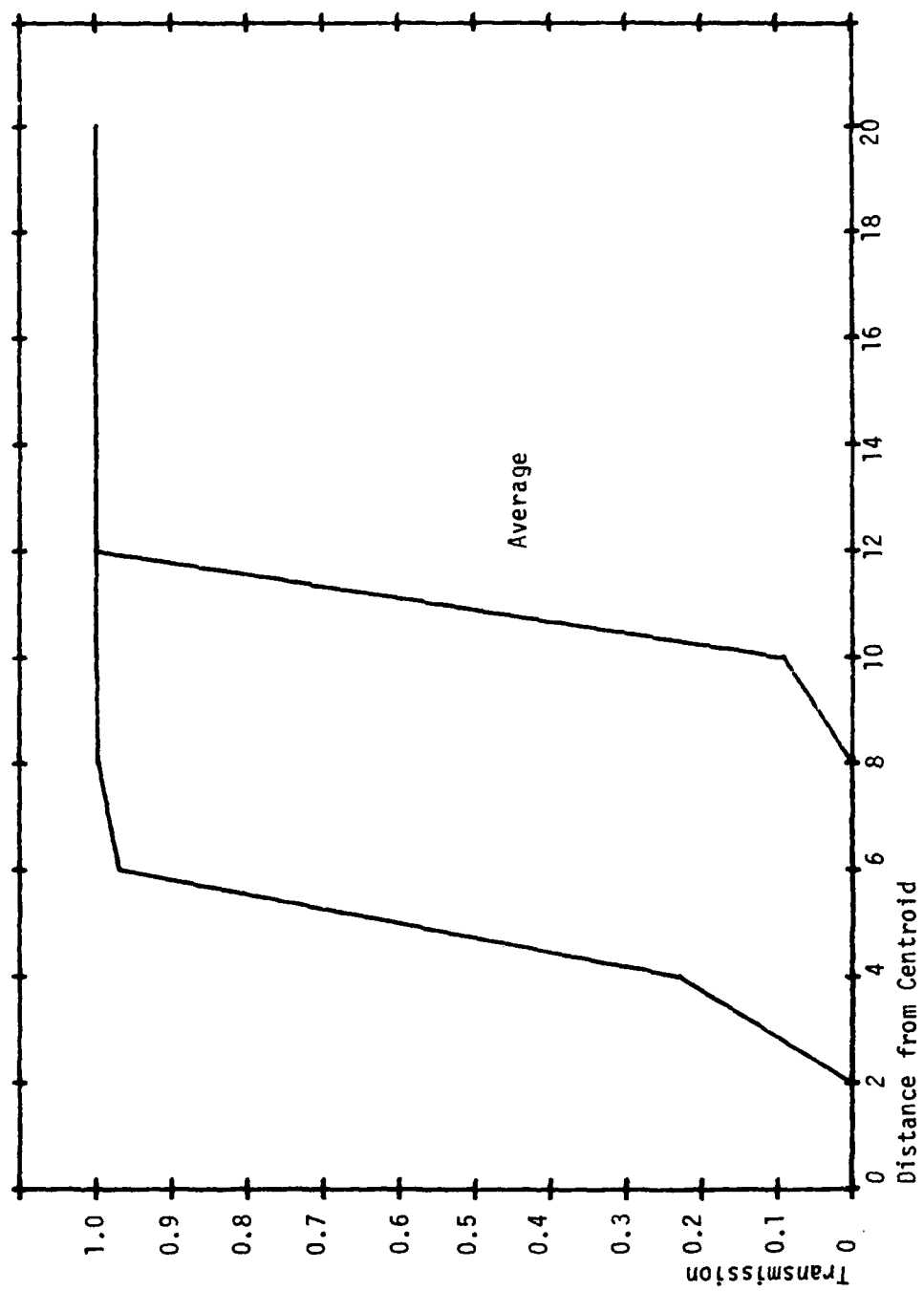


Figure 58. Transmission versus distance, second moment average, time  $T_2$ ,  
 $n(r) = 1/r^2$ .

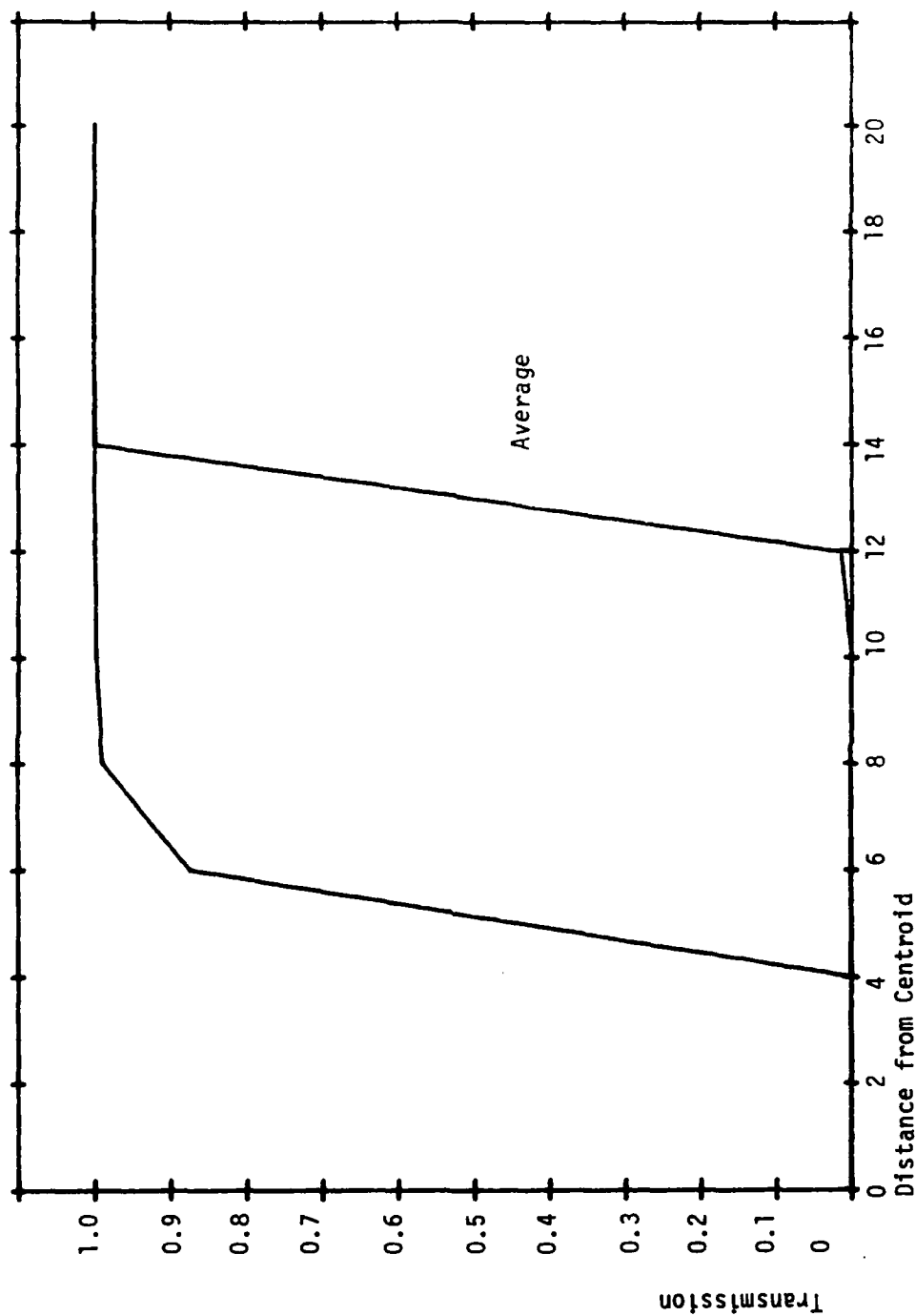


Figure 59. Transmission versus distance, second moment average, time  $T_3$ ,  $n(r) = 1/r^3$ .

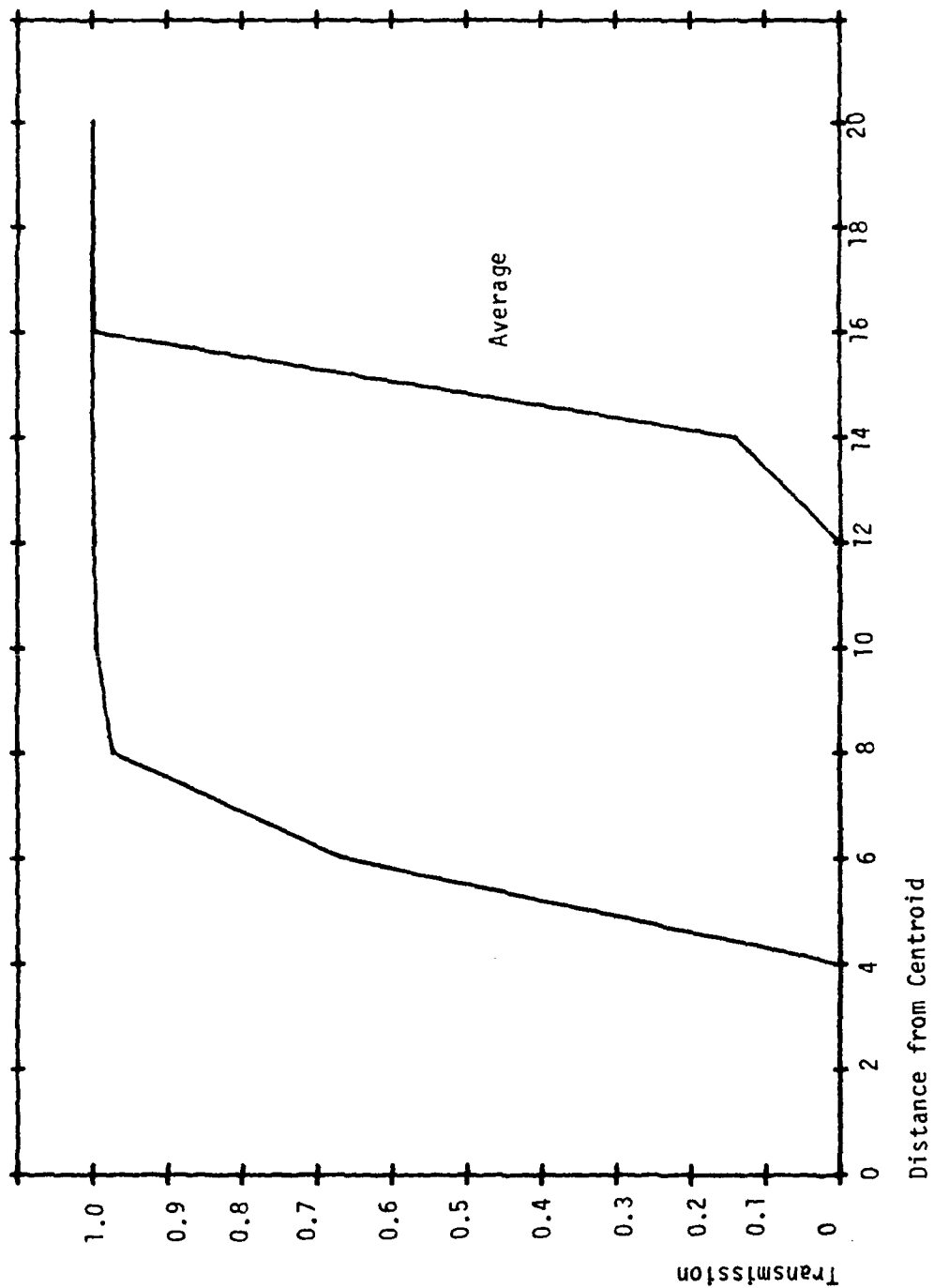


Figure 60. Transmission versus distance, second moment average, time  $T_4$ ,  
 $n(r) \approx 1/r^3$ .

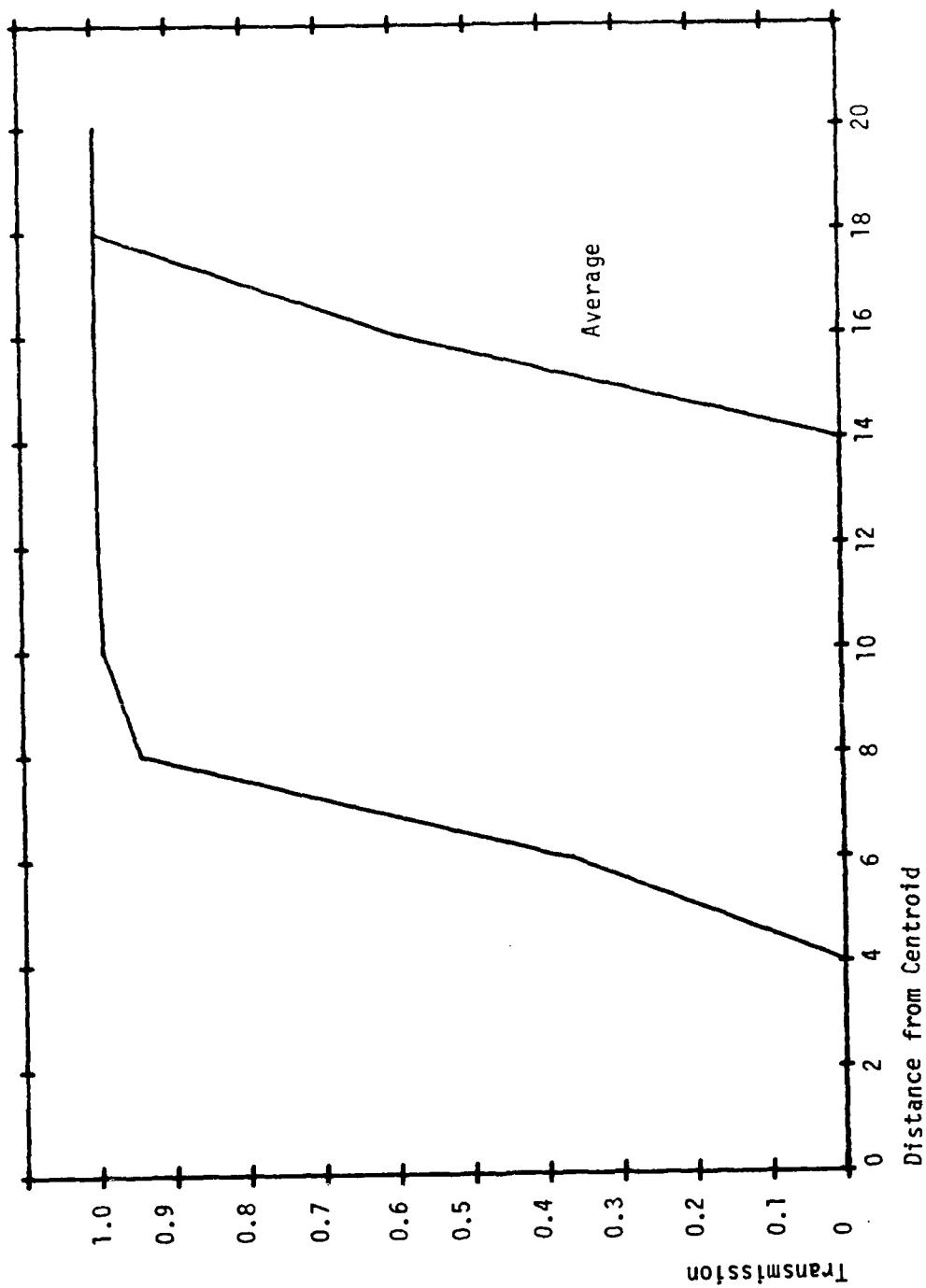


Figure 61. Transmission versus distance, second moment average, time  $T_5$ ,  
 $n(r) = 1/r^3$ .

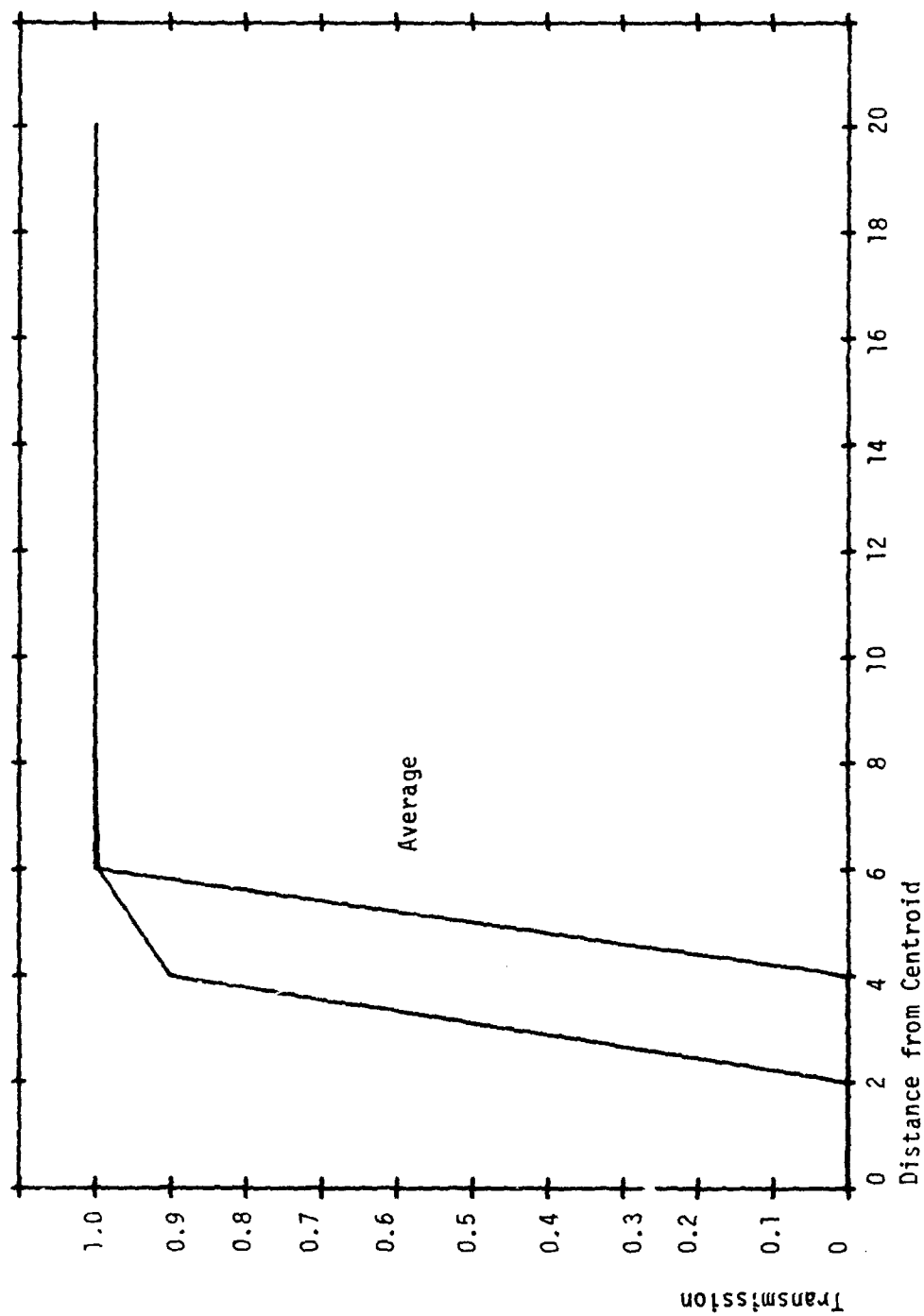


Figure 62. Transmission versus distance, third moment average, time  $T_1$ ,  
 $n(r) = 1/r^3$ .

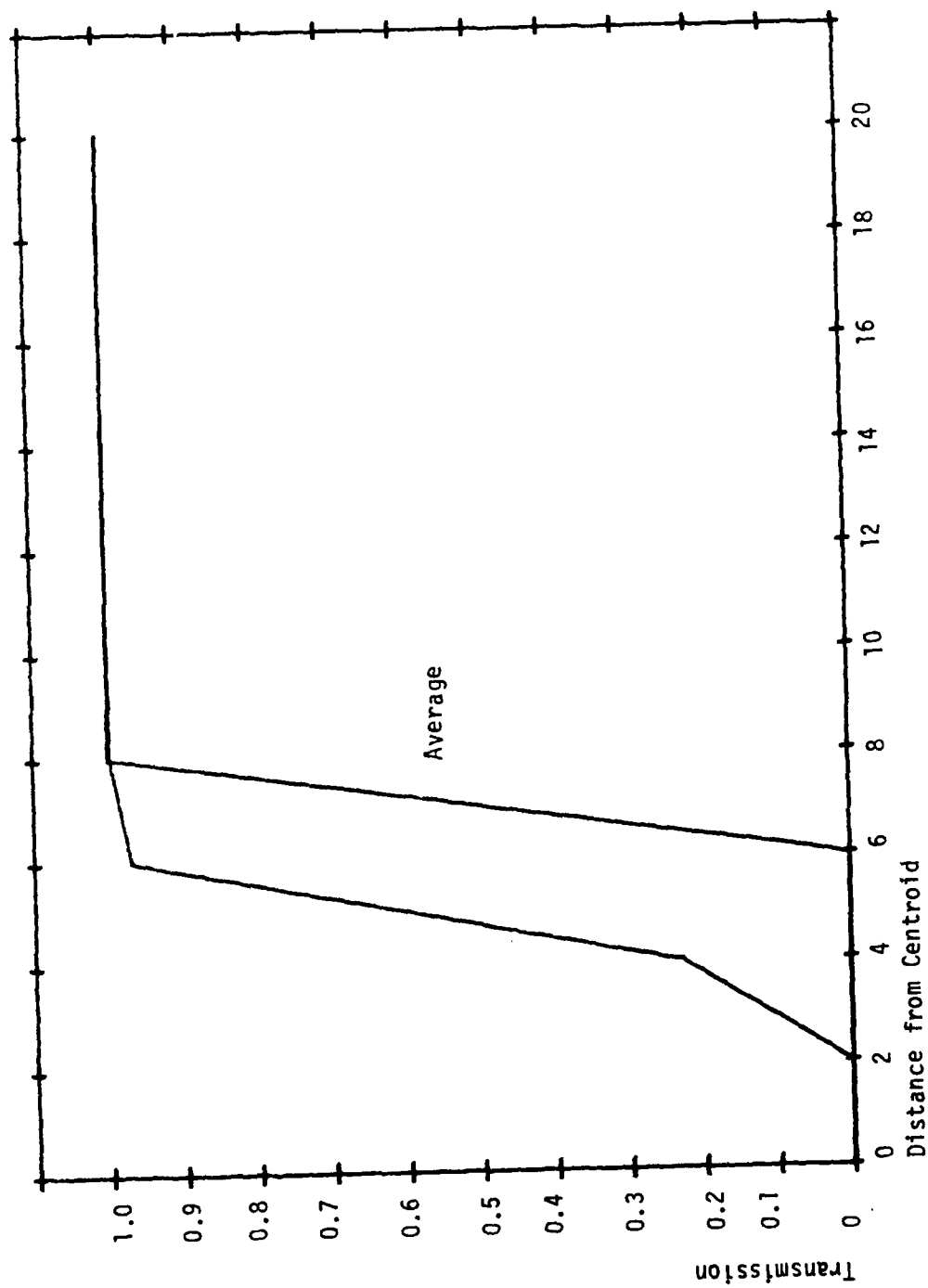


Figure 63. Transmission versus distance, third moment average, time  $T_2$ ,  
 $n(r) = 1/r^3$ .

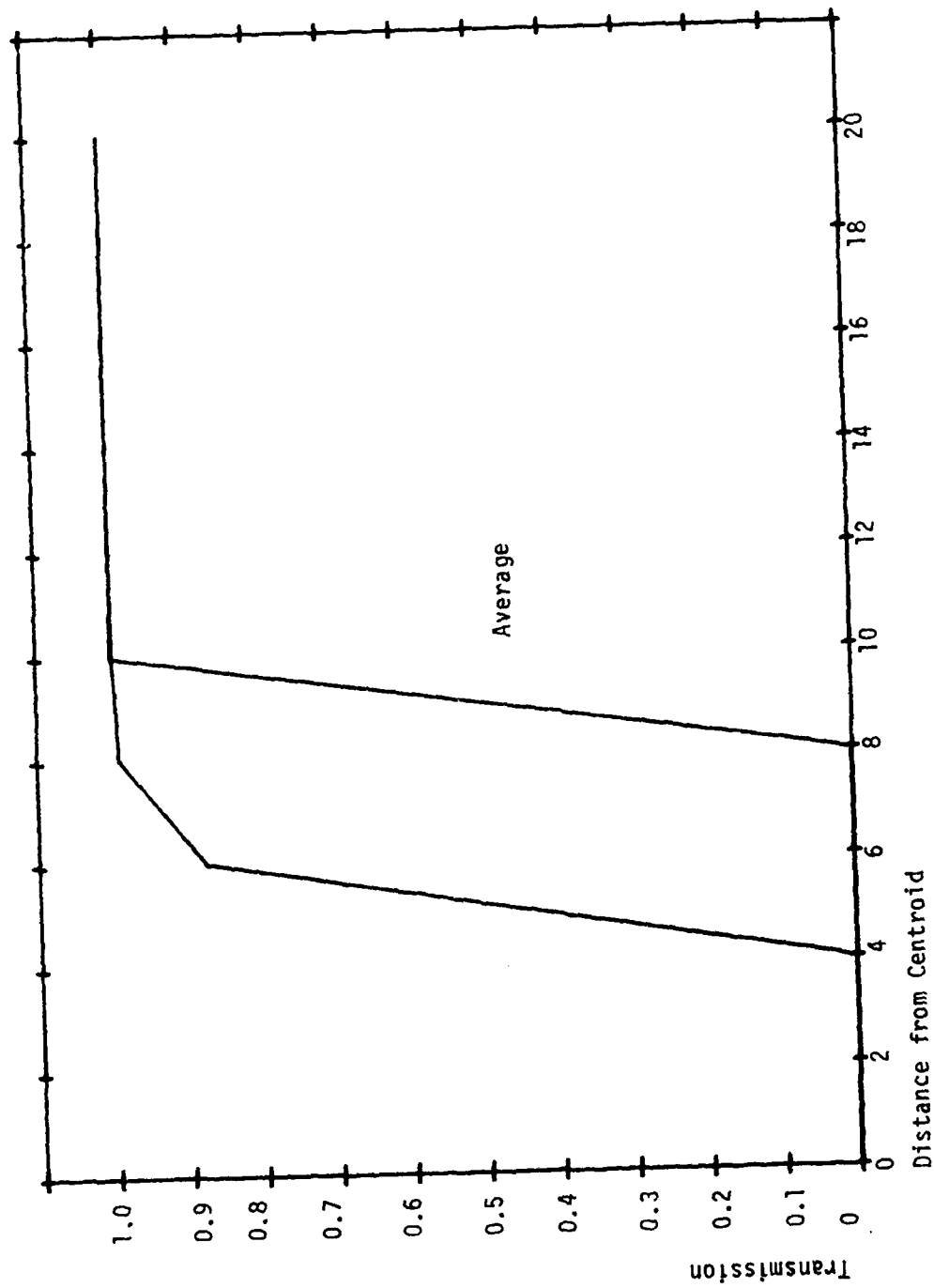


Figure 64. Transmission versus distance, third moment average, time  $T_3$ ,  
 $n(r) = 1/r^3$ .

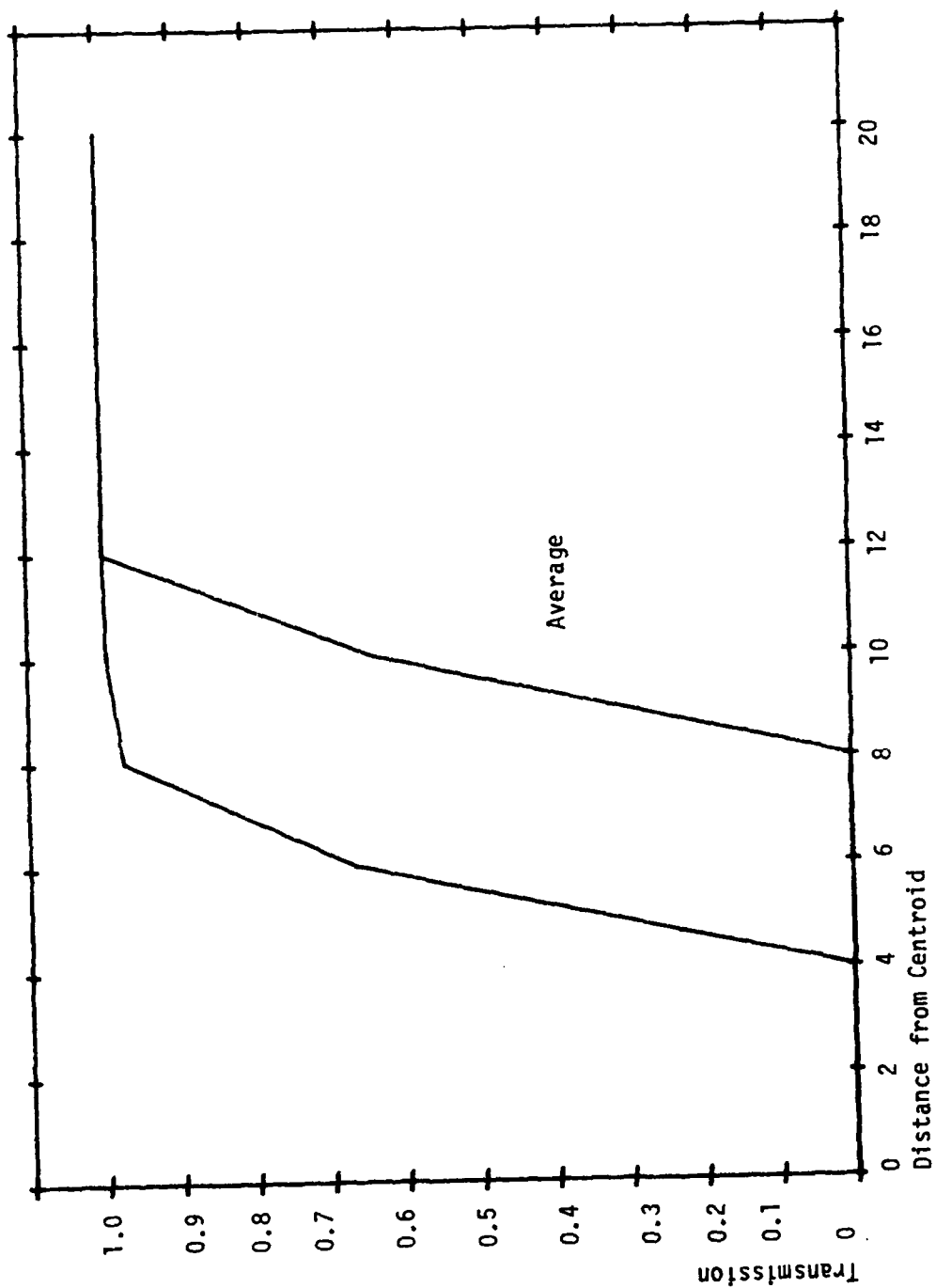


Figure 65. Transmission versus distance, third moment average, time  $T_4$ ,  
 $n(r) = 1/r^3$ .

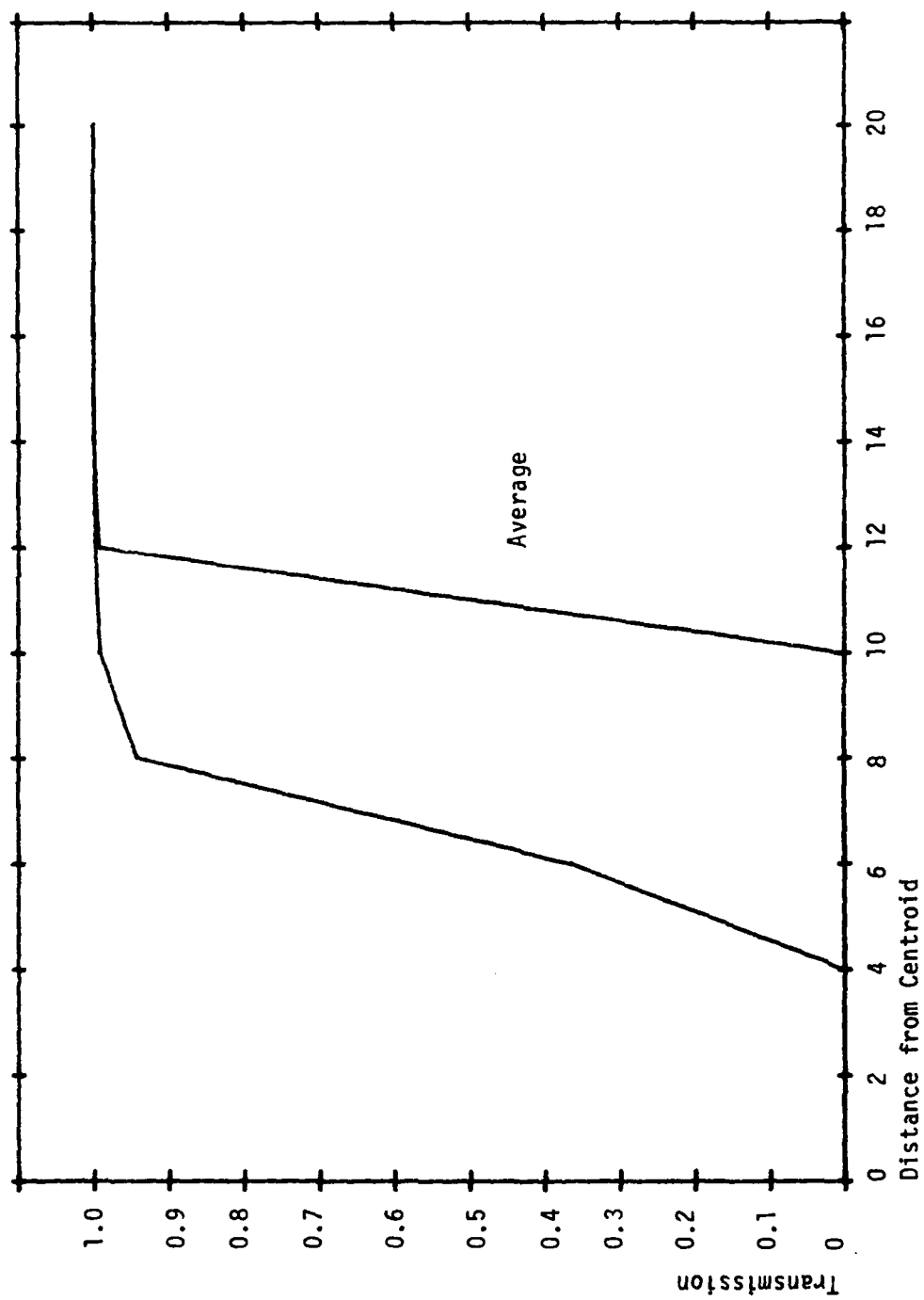


Figure 66. Transmission versus distance, third moment average, time  $T_5$ ,  
 $n(r) = 1/r^3$ .

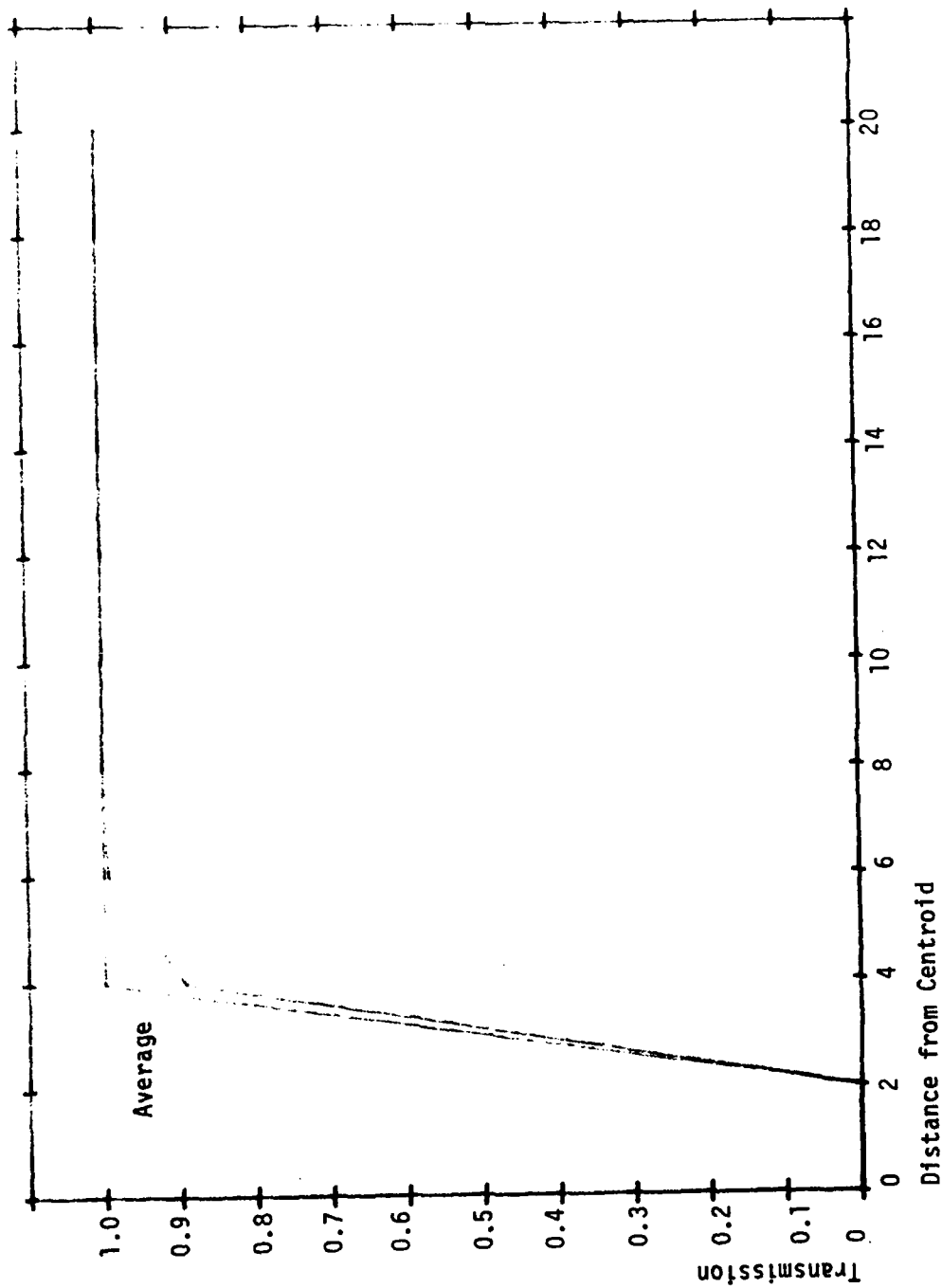


Figure 67. Transmission versus distance, first moment average, time  $T_1$ ,  
 $n(r)$  = Deirmendjian haze H.

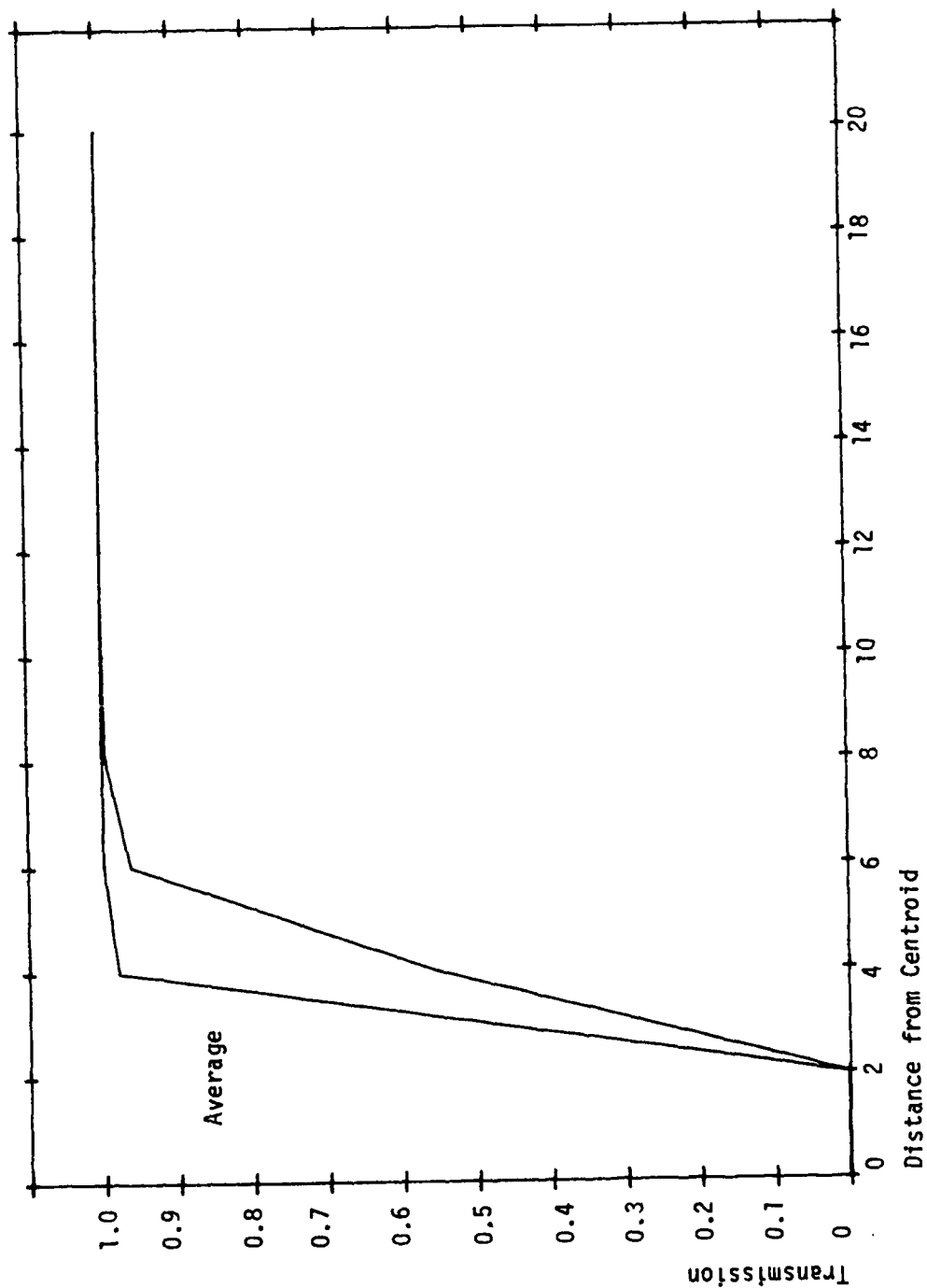


Figure 68. Transmission versus distance, first moment average, time  $T_2$ .  
 $n(r)$  = Deirmendjian haze H.

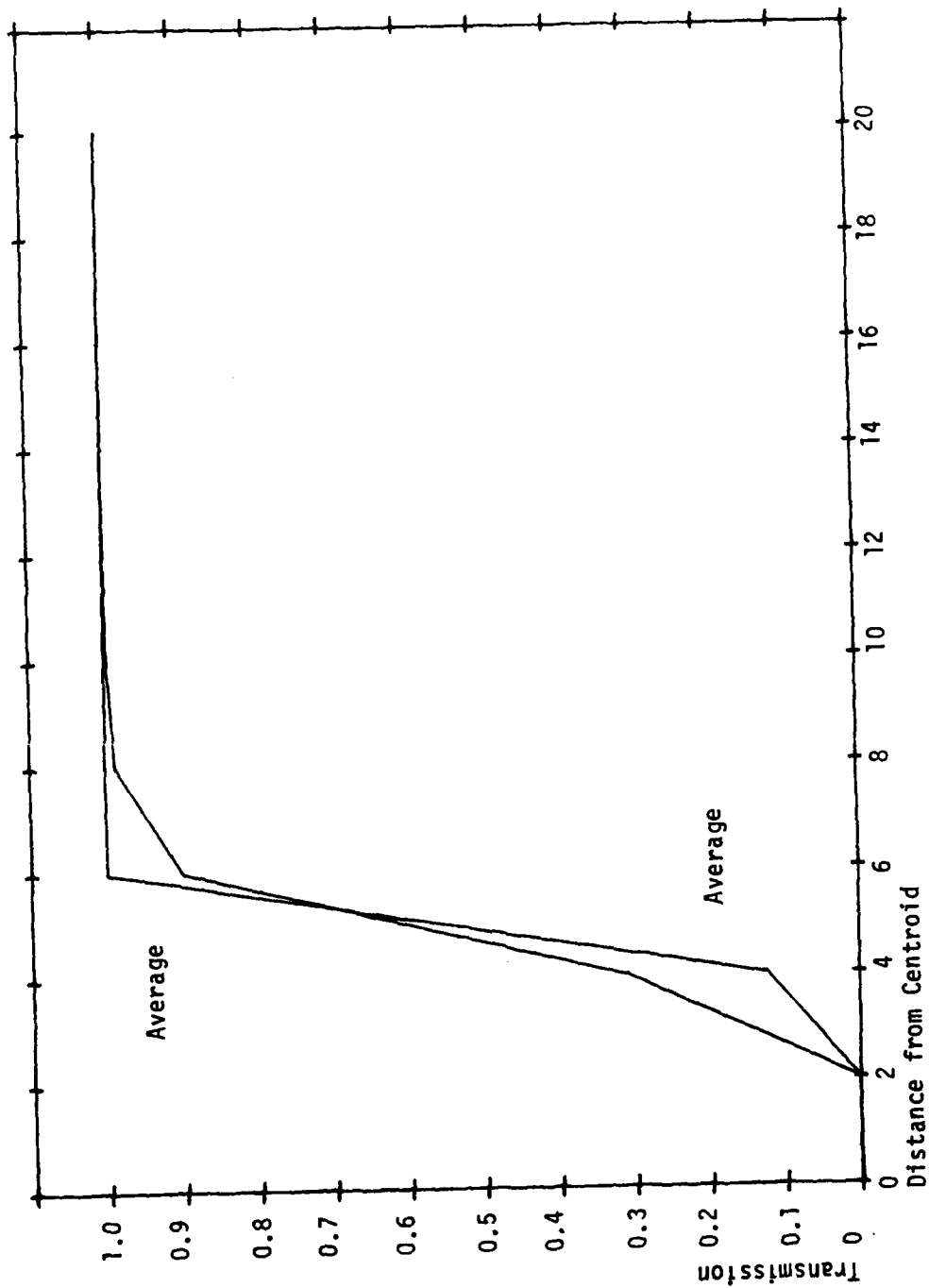


Figure 69. Transmission versus distance, first moment average, time T<sub>3</sub>,  
 $n(r) \approx$  Deirmendjian haze H.

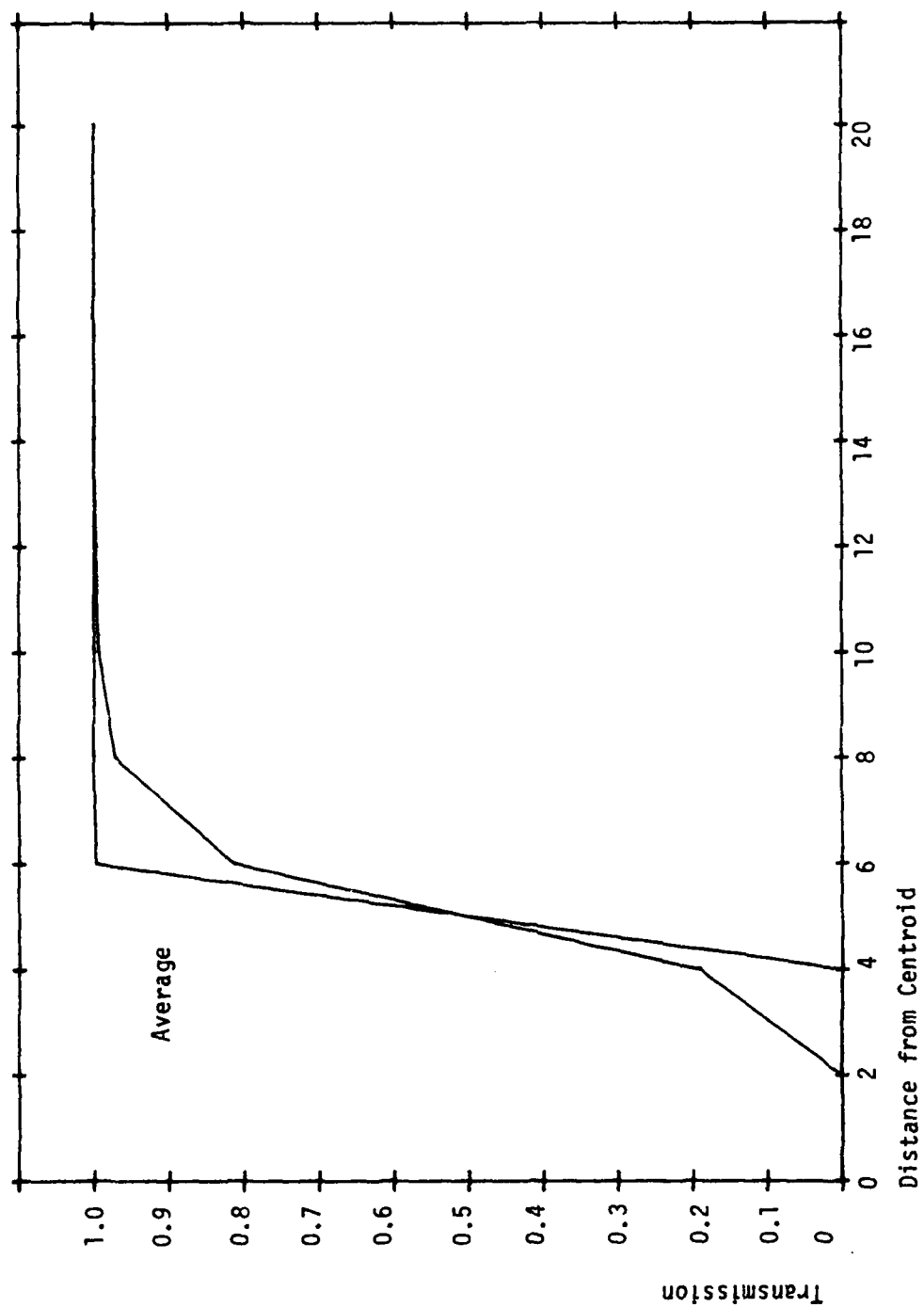


Figure 70. Transmission versus distance, first moment average, time  $T_4$ ,  $n(r)$  = Deirmendjian haze H.

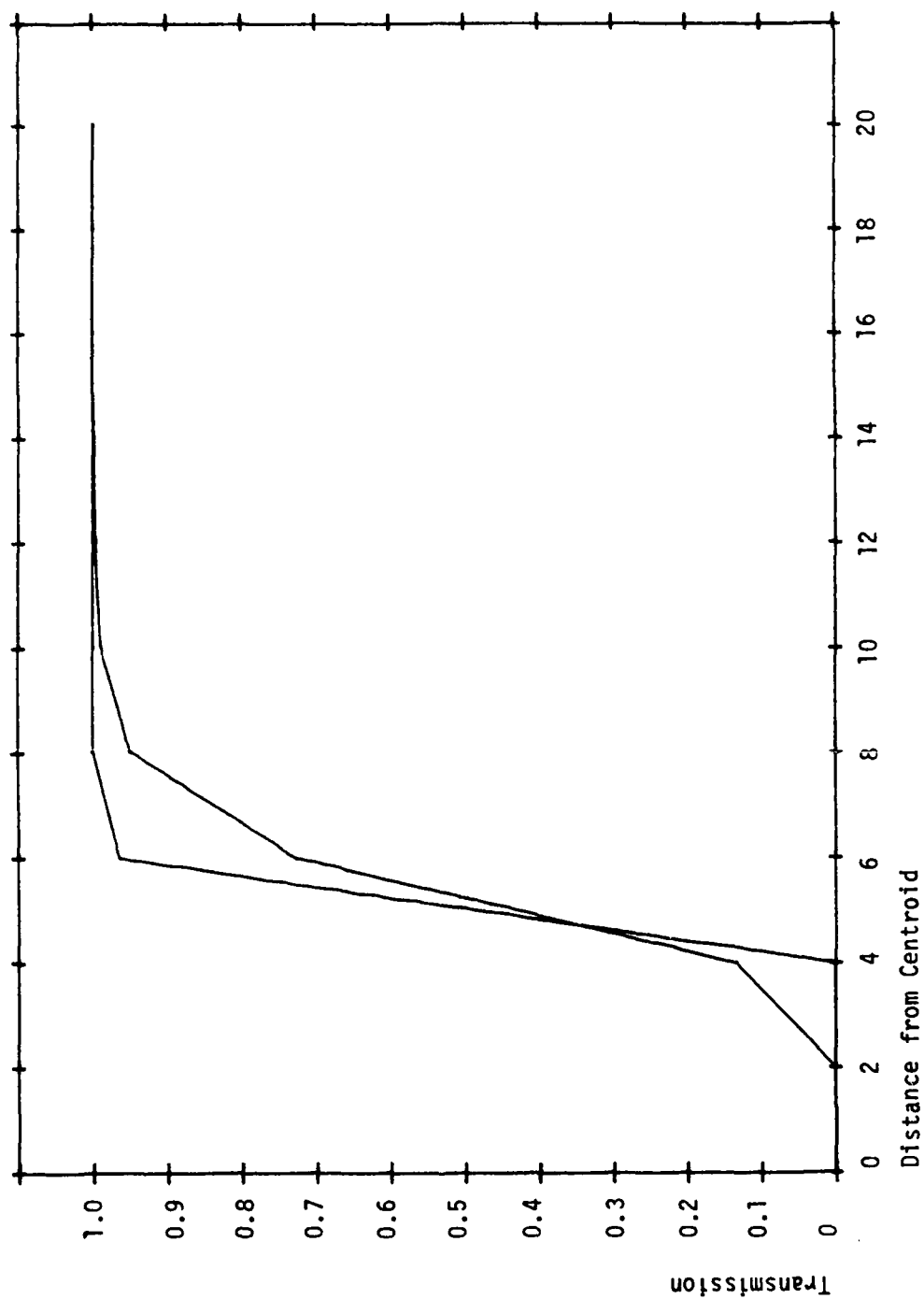


Figure 71. Transmission versus distance, first moment average, time  $T_5$ ,  
 $n(r)$  = Deirmendjian haze H.

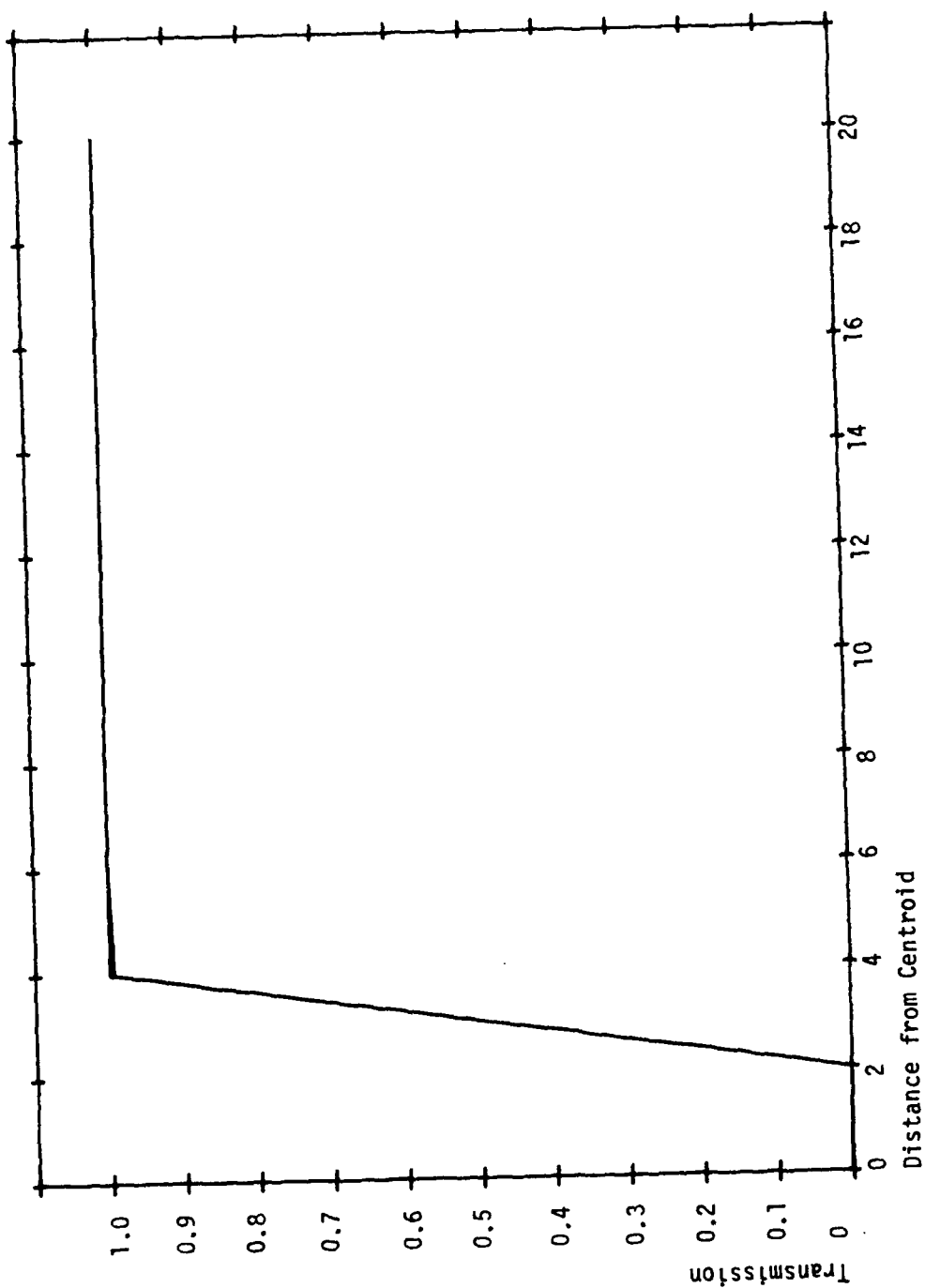


Figure 72. Transmission versus distance, second moment average, time  $T_1$ ,  
 $n(r)$  = Deirmendjian haze H.

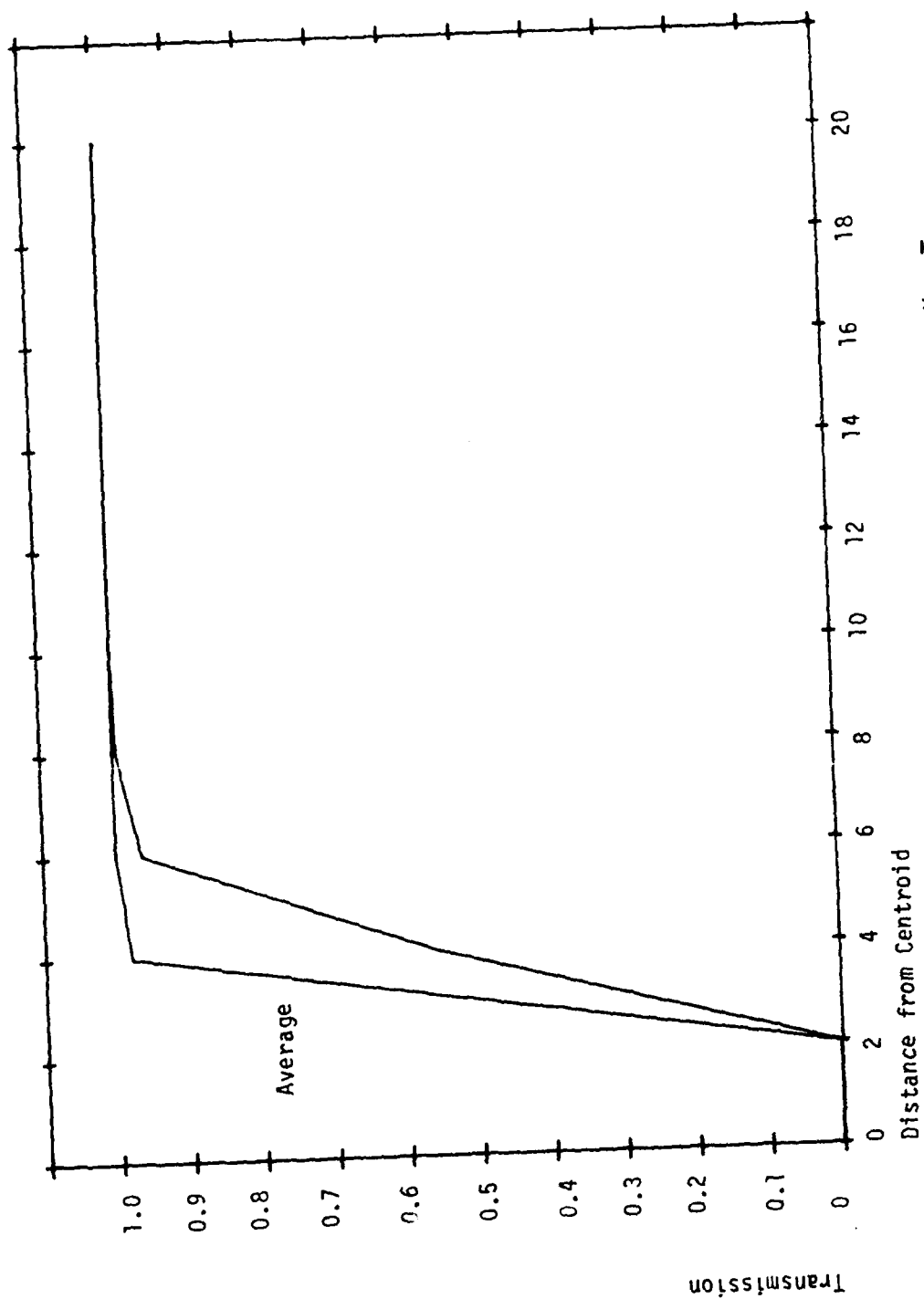


Figure 73. Transmission versus distance, second moment average, time  $T_2$ .  
 $n(r) = \text{Deirmendjian haze } H.$

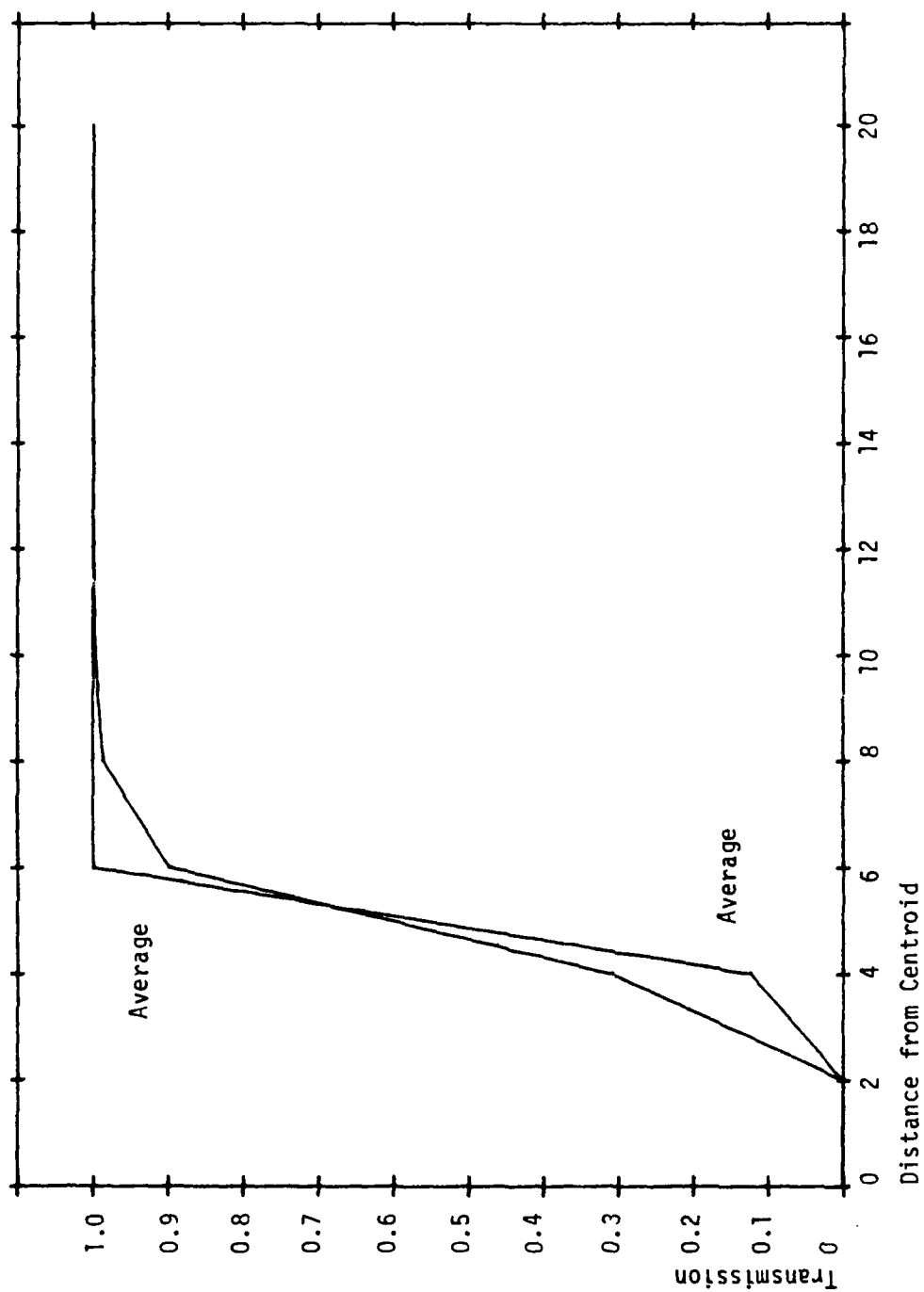


Figure 74. Transmission versus distance, second moment average, time  $T_3$ ,  
 $n(r)$  = Deirmendjian haze H.

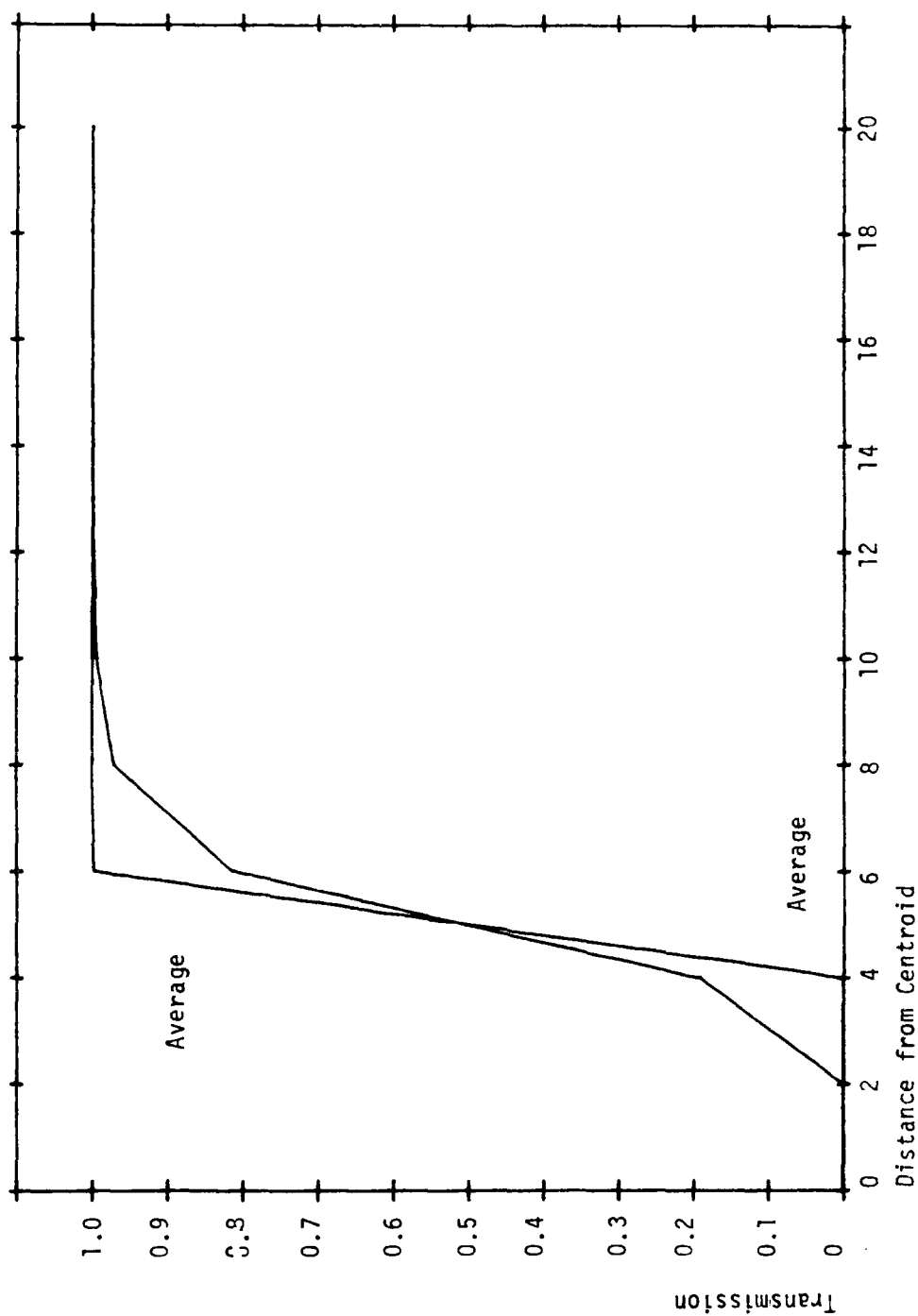


Figure 75. Transmission versus distance, second moment average, time  $T_4$ ,  
 $n(r)$  = Deirmendjian haze H.

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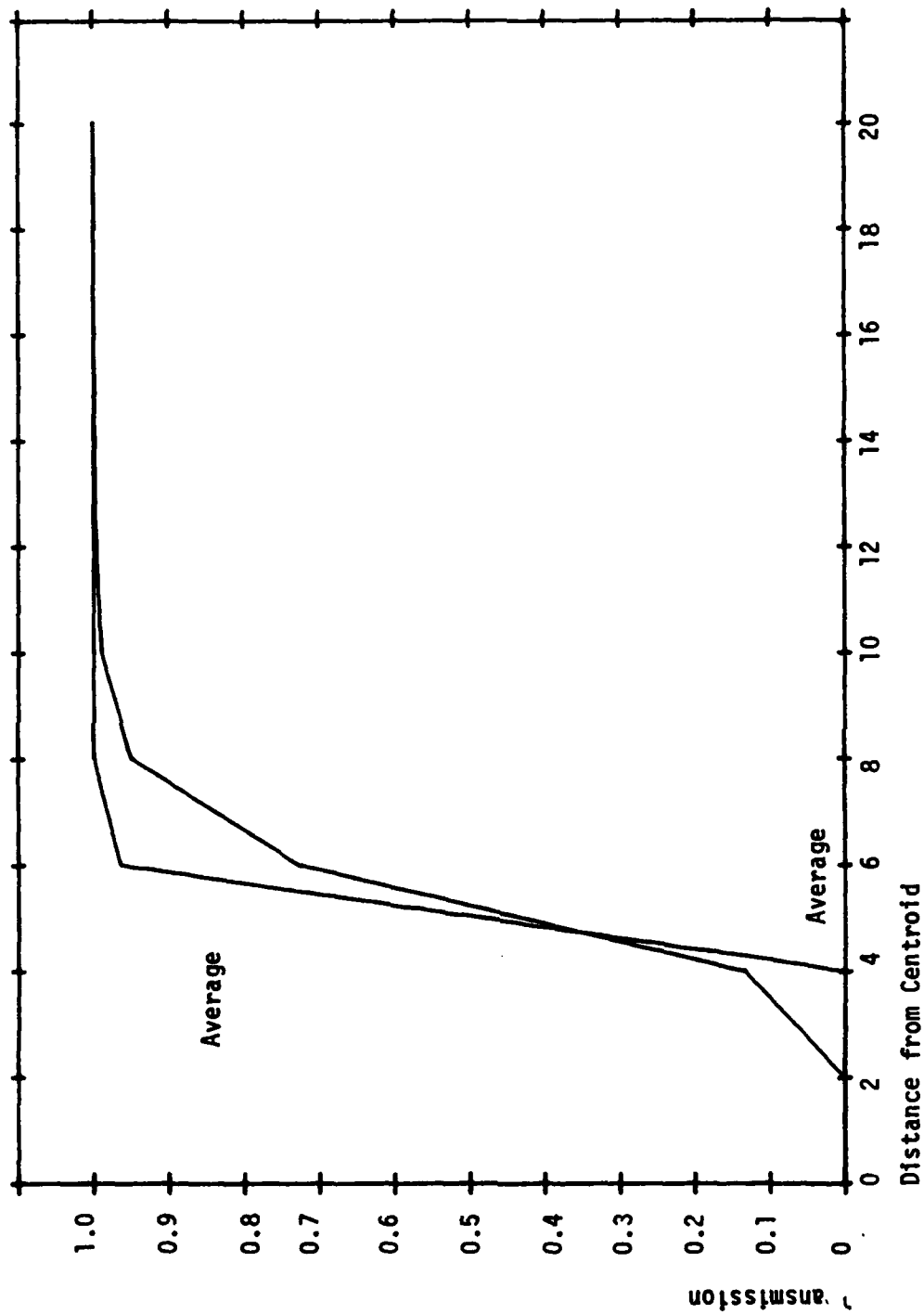


Figure 76. Transmission versus distance, second moment average, time T5,  
 $n(r)$  = Deirmendjian haze H.

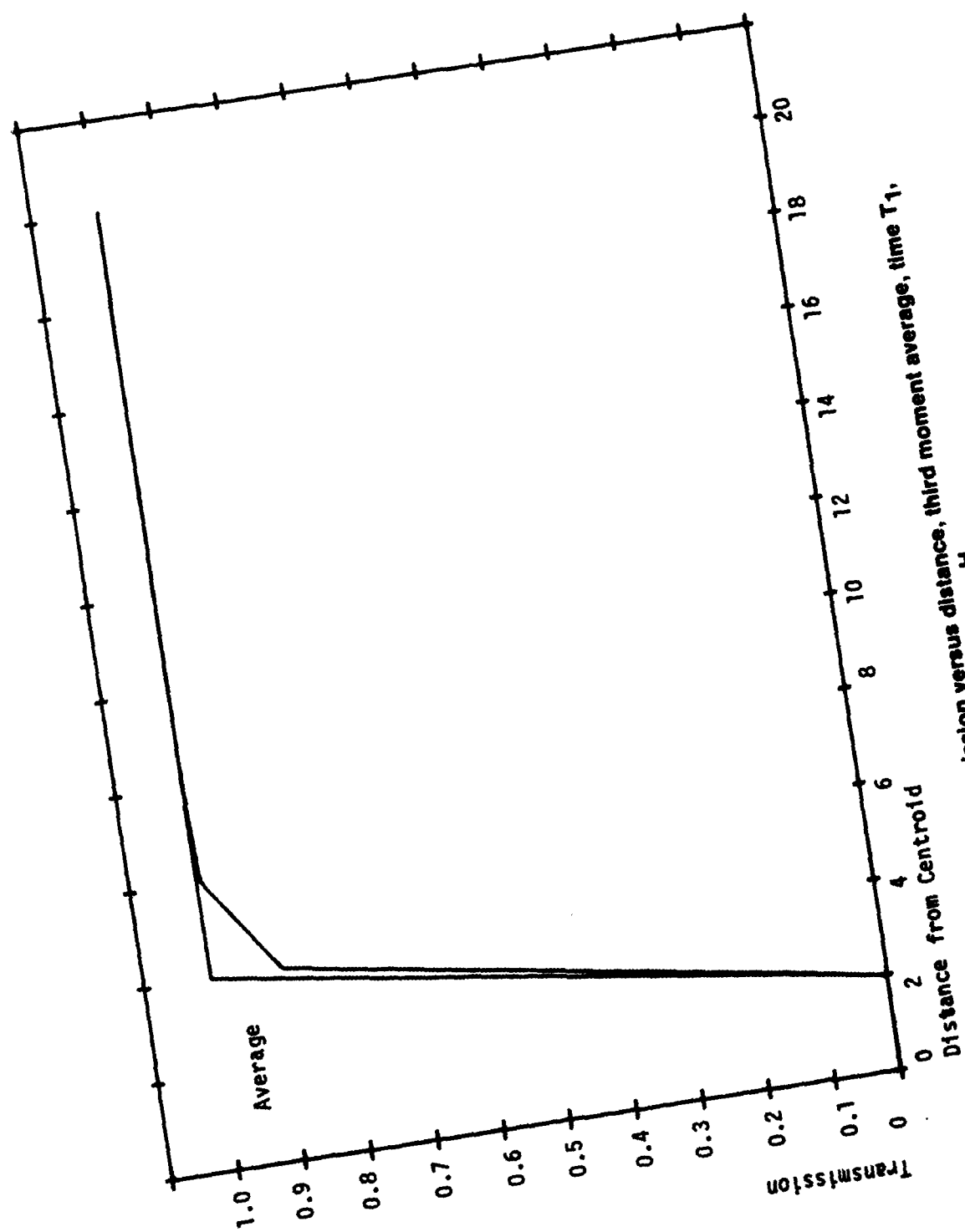


Figure 77. Transmission versus distance, third moment average, time  $T_1$ ,  $n(r) = \text{Deirmendjian haze H.}$

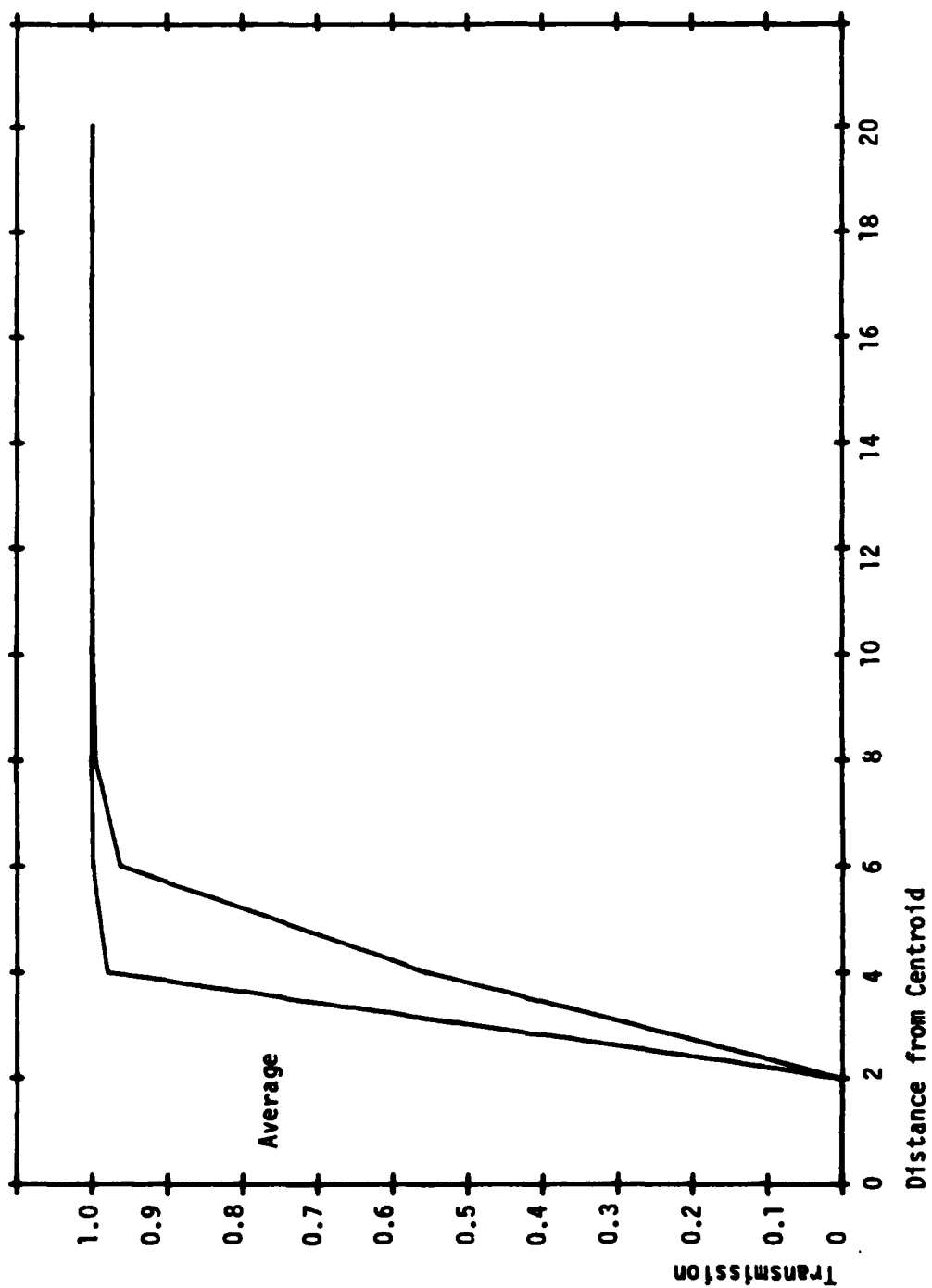


Figure 78. Transmission versus distance, third moment average, time  $T_2$ .  
 $n(r)$  = Delmendjian haze H.

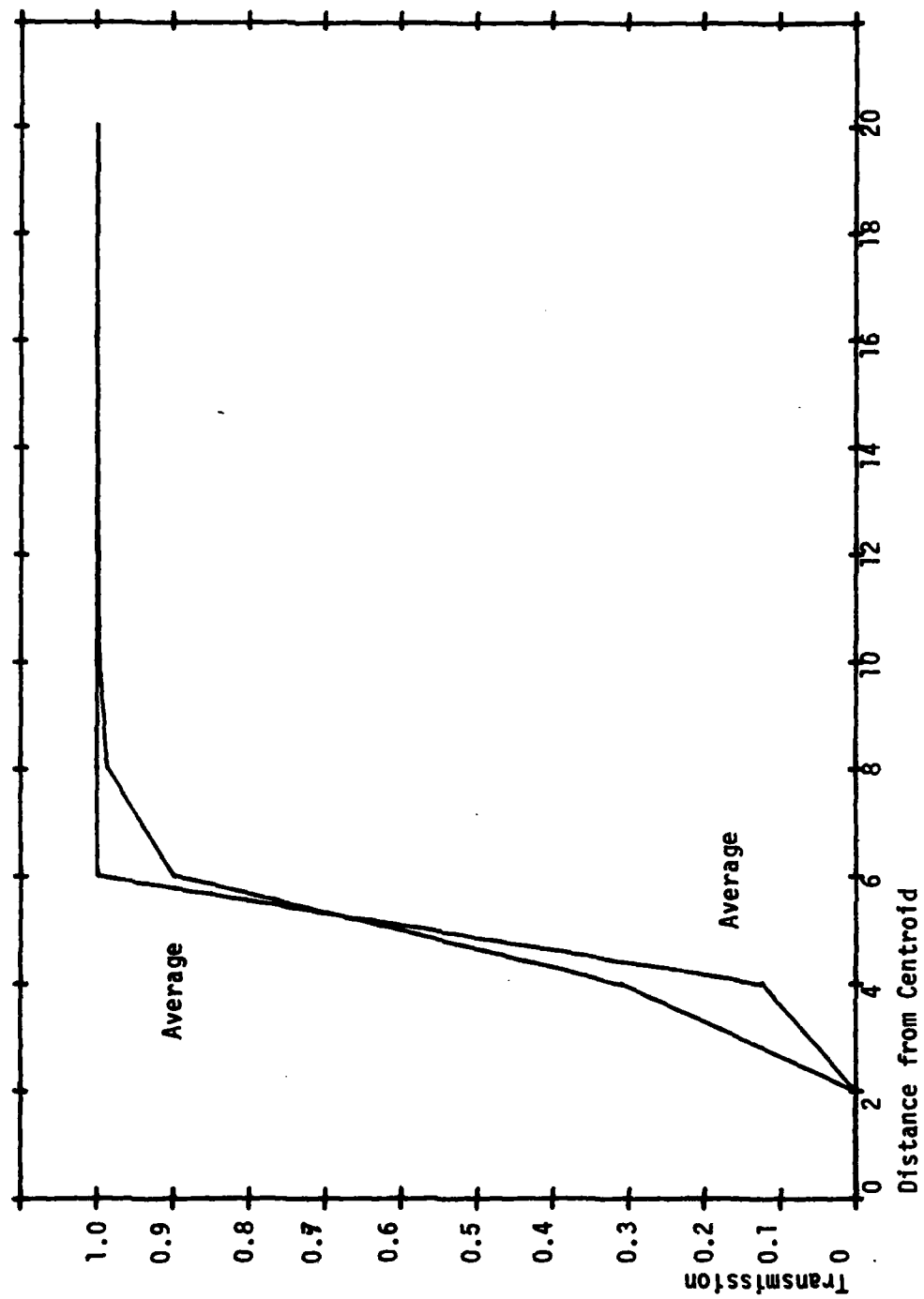


Figure 79. Transmission versus distance, third moment average, time  $T_3$ ,  
 $n(r)$  = Deirmendjian haze H.

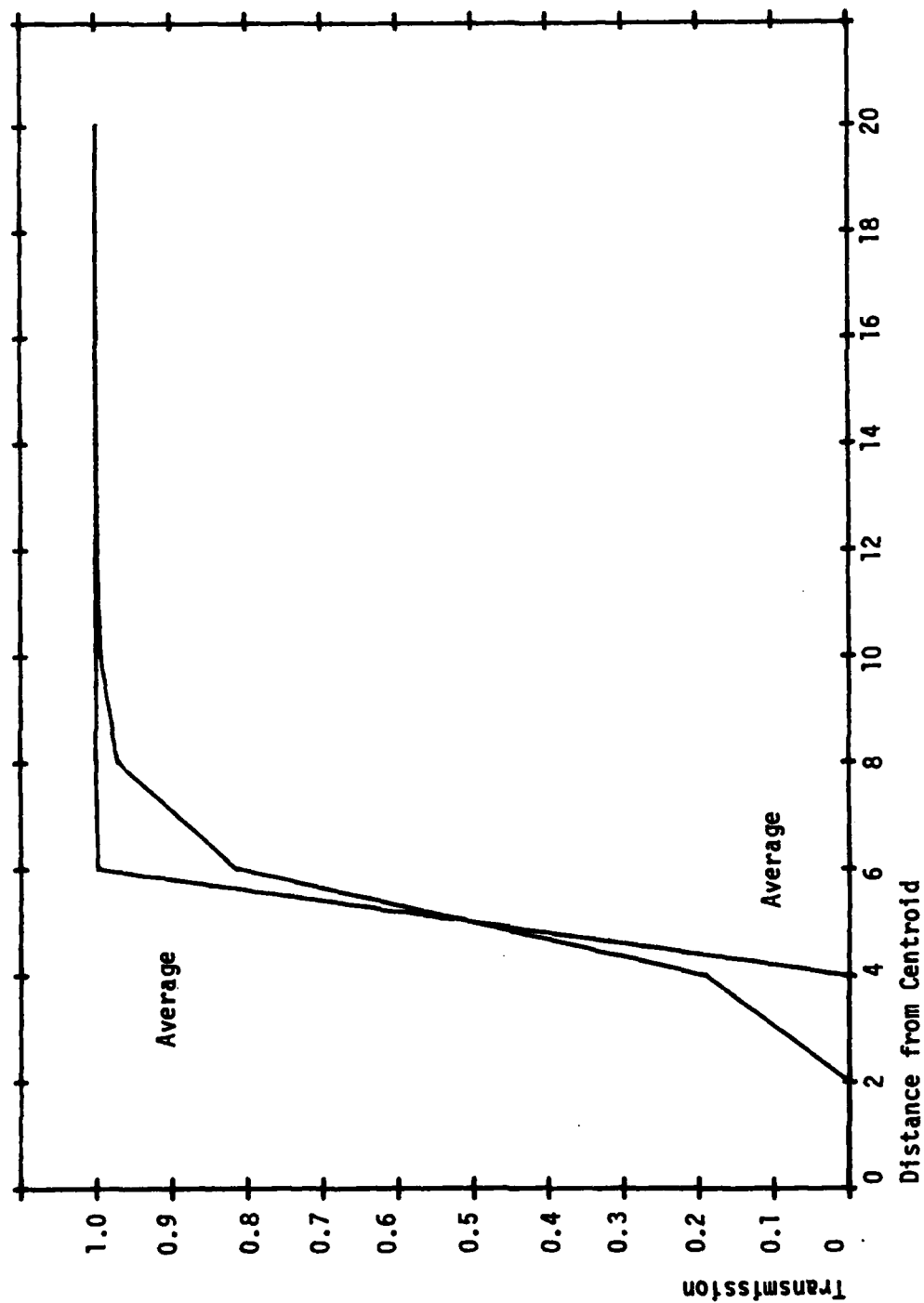


Figure 80. Transmission versus distance, third moment average, time  $T_4$ ,  
 $n(r)$  = Deirmendjian haze H.

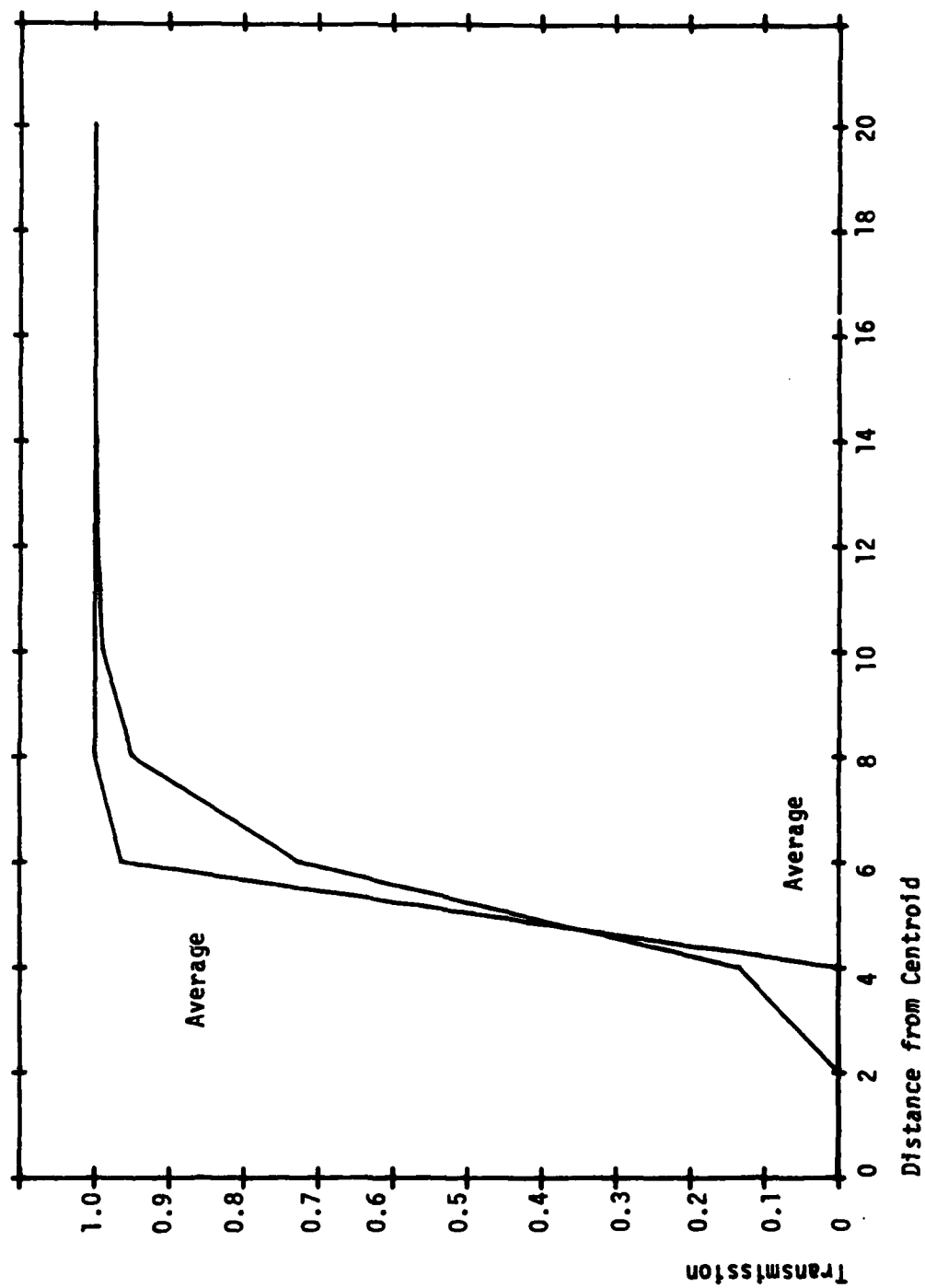


Figure 81. Transmission versus distance, third moment average, time T5.  
 $n(r)$  = Deirmendjian haze H.

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